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(54) Title: METHOD OF IDENTIFYING INHIBITORS OF TIE-2

(57) Abstract: The present invention relates to polypeptides which comprise the ligand binding domain of Tie-2, crystalline forms of these polypeptides and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Tie-2. The invention also relates to the use of the three dimensional structure of the Tie-2 catalytic domain both alone, or in complex with inhibitors, in methods of designing and/or identifying potential inhibitors of Tie-2 activity, for example, compounds which inhibit the binding of a native substrate to the Tie-2 catalytic domain.

METHOD OF IDENTIFYING INHIBITORS OF TIE-2

RELATED APPLICATION

This application claims the benefit of U.S. Provisional Application No. 60/192,920, filed on March 29, 2000. The entire teachings of the above application is incorporated herein by reference.

BACKGROUND OF THE INVENTION

Angiogenesis is a fundamental process by which new blood vessels are formed through sprouting, branching, proliferation, and tubule formation by endothelial cells from existing vasculature. In healthy humans, this neovascularization is under stringent control, normally occurring only during embryonic development, endometrial regulation, breast lactation and wound repair. However, in many pathological conditions, such as rheumatoid arthritis, solid tumors, Kaposi's sarcoma, blindness due to ocular neovascularization, psoriasis and atherosclerosis, disease progression is dependent upon persistent angiogenesis. The vasculature, which is the conduit for drug delivery, is one of the most accessible tissues in the body. Each endothelial cell of tumor vessels is estimated to support 100 to 1,000 neighboring cells, yet in the absence of an angiogenic stimulus endothelial cells typically divide only once every thousand days.

A number of polypeptide growth factors and their associated endothelial cell specific receptors have been discovered which are primarily responsible for the stimulation of endothelial cell growth, differentiation and the establishment of new vasculature. These growth factor receptors include the vascular endothelial growth factor receptors (VEGFR) Flk-1 (mouse), KDR/VEG-FR-2 (human), Flt-1/VEGFR-1, and Flt-4/VEGFR-3. Receptors which are responsible for neovascularizaton also include the receptor tyrosine kinases Tie-1 and Tie-2.

Due to its role in regulating new vascular development, Tie-2 is a potential target for therapies aimed at controlling diseases which depend upon persistent angiogenesis. The development of biochemical assays for Tie-2 has enabled drug

discovery to proceed along the pathways of identifying lead Tie-2 inhibitors by high-throughput screening of compound libraries and by testing compounds that mimic substrate structure; however, rational, structure-based design has not been possible up to this point because of the lack of accurate three-dimensional structural data for Tie-2 receptors.

SUMMARY OF THE INVENTION

The present invention relates to a polypeptide which comprises the catalytic domain of Tie-2, a crystalline form of this polypeptide and the use of structural information derived from the crystalline form of the polypeptide for designing and/or identifying potential inhibitors of the binding of one or more native ligands to the catalytic domain of Tie-2.

In one embodiment, the present invention relates to a polypeptide comprising the catalytic domain of TIE-2 and having the amino acid sequence set forth in SEQ ID NO: 2. In another embodiment, the invention relates to a crystalline form of this polypeptide or the polypeptide complexed with a ligand.

In another embodiment, the invention provides a method of determining the three dimensional structure of a crystalline polypeptide comprising the Tie-2 catalytic domain. In one embodiment, the method comprises the steps of (1) obtaining a crystal of the polypeptide comprising the catalytic domain of Tie-2; (2) obtaining x-ray diffraction data for said crystal; and (3) solving the crystal structure of said crystal. The method optionally comprises the additional step of obtaining the polypeptide, with the three dimensional structure to be determined, prior to obtaining the crystal of said peptide.

In another embodiment, the method comprises the steps of (1) obtaining a crystal of the polypeptide comprising the catalytic domain of Tie-2; (2) obtaining x-ray diffraction data for said crystal; and (3) solving the crystal structure of said crystal by using said x-ray diffraction data and the atomic coordinates for the Tie-2 catalytic domain of a second polypeptide. The method optionally comprises the additional step of obtaining the polypeptide, with the three dimensional structure to be determined, prior to obtaining the crystal of said peptide.

The invention further relates to a method for identifying a compound which inhibits the catalytic activity of Tie-2 by, for example, inhibiting the binding of natural substrates such as a tyrosyl polypeptide or protein or ATP, to the catalytic domain of Tie-2. Such a compound is referred to herein as a "Tie-2 inhibitor". The method comprises the steps of (1) using a three-dimensional structure of Tie-2 as defined by the atomic coordinates of the cataytic domain of Tie-2; (2) employing the three dimensional structure to design or select a potential inhibitor; and (3) assessing the ability of the selected compound to inhibit the catalytic activity of Tie-2 . The method can also include the step of providing the compound designed or selected in step 2, for example, by synthesizing the compound or obtaining the compound from a compound library. In addition, the method can include the step of assessing the ability of the identified compound to bind to the catalytic domain of Tie-2 and/or assessing the ability of the identified compound to inhibit the binding of a natural ligand of Tie-2.

In another embodiment, the method for identifying a compound which inhibits the catalytic activity of Tie-2, comprises the step of determining the ability of one or more functional groups and/or moieties of the compound, when present in, or bound to, the Tie-2 catalytic domain, to interact with one or more subsites of the Tie-2 catalytic domain. Generally, the Tie-2 catalytic domain is defined by the conserved homologous seqences when compared to other known tyrosine kinases. If the compound is able to interact with a preselected number or set of subsites, or has a calculated interaction energy within a desired or preselected range, the compound is identified as a potential inhibitor of Tie-2.

The invention further provides a method of designing a compound which is a potential inhibitor of the catalytic activity of Tie-2. The method includes the steps of (1) identifying one or more functional groups capable of interacting with one or more subsites of the Tie-2 catalytic domain; and (2) identifying a scaffold which presents the functional group, or functional groups, identified in step 1 in a suitable orientation for interacting with one or more subsites of the Tie-2 catalytic domain. The compound which results from attachment of the identified functional groups or moieties to the identified scaffold is a potential inhibitor of Tie-2. The Tie-2 catalytic

domain is, generally, defined by the atomic coordinates of a polypeptide comprising the Tie-2 catalytic domain.

In yet another embodiment, the invention provides compounds which inhibit the catalytic activity of Tie-2 and which fit, or bind to, the Tie-2 catalytic domain. Such compounds typically comprise one or more functional groups which, when the compound is bound in the Tie-2 catalytic domain, interact with one or more subsites of the catalytic domain. Generally, the Tie-2 catalytic domain is defined by the conserved homologous sequence when compared to other known tyrosine kinases. In a particular embodiment, the Tie-2 inhibitor is a compound which is identified or designed by a method of the present invention.

The present invention further provides a method for treating a condition mediated by Tie-2 in a patient. The method comprises administering to the patient a therapeutically or prophylactically effective amount of a compound which inhibits the catalytic activity of Tie-2, such as a Tie-2 inhibitor of the invention, for example, a compound identified as a Tie-2 inhibitor or designed to inhibit Tie-2 by a method of the present invention.

The present invention provides several advantages. For example, the invention provides the first detailed three dimensional structures of the ligand binding domain of a Tie-2 protein. The methods described herein can be used to facilitate formation of Tie-2 crystals which diffract at high resolution. These structures enable the rational development of inhibitors of Tie-2 by permitting the design and/or identification of molecular structures having features which facilitate binding to the Tie-2 binding domain. The methods of use of the structures disclosed herein, thus, permit more rapid discovery of compounds which are potentially useful for the treatment of conditions which are mediated, at least in part, by Tie-2 activity.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 presents the amino acid sequence of human Tie-2 (SEQ ID NO: 1).

Fig. 2 presents the amino acid sequence which includes the catalytic domain of human Tie-2 from amino acid 802 to amino acid 1124, and has a catalytically inactive point mutation at amino acid 964 (SEQ ID NO: 2).

Fig. 3A-3OO present the atomic coordinates for SEQ ID NO 2/inhibitor I complex.

Fig. 4A-4OO present the atomic coordinates for SEQ ID NO 2/inhibitor II complex.

Fig. 5A-5RR present the atomic coordinates for SEQ ID NO 2/inhibitor III complex.

Fig. 6A-6NN present the atomic coordinates for SEQ ID NO 2/inhibitor IV complex.

Fig. 7 shows the structure of a prototypical kinase, insulin receptor kinase.

Fig. 8 shows identifies regions of a pyrrolopyrimidine inhibitor (i.e., inhibitor I) which interact with the catalytic domain of Tie-2.

Fig. 9 shows a model of the catalytic domain of Tie-2 bound to inhibitor I. Subsites are shown in different colors.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the x-ray crystallographic study of polypeptides comprising the catalytic domain of Tie-2. The atomic coordinates which result from this study are of use in identifying compounds which fit in the catalytic domain and are, therefore, potential inhibitors of Tie-2. These Tie-2 inhibitors are of use in methods of treating a patient having a condition which is modulated by or dependent upon Tie-2 activity, for example, a condition dependent on persistant angiogenesis.

There are at least 400 enzymes identified as protein kinases. These enzymes catalyze the phosphorylation of target protein substrates. The phosphorylation is usually a transfer reaction of a phosphate group from ATP to the protein substrate. The specific structure in the target substrate to which the phosphate is transferred is a tyrosine, serine or threonine residue. Since these amino acid residues are the target structures for the phosphoryl transfer, these protein kinase enzymes are commonly referred to as tyrosine kinases or serine/threonine kinases.

The phosphorylation reactions, and counteracting phosphatase reactions, at the tyrosine, serine and threonine residues are involved in countless cellular processes that

underlie responses to diverse intracellular signals (typically mediated through cellular receptors), regulation of cellular functions, and activation or deactivation of cellular processes. A cascade of protein kinases often participate in intracellular signal transduction and are necessary for the realization of these cellular processes. Because of their ubiquity in these processes, the protein kinases can be found as an integral part of the plasma membrane or as cytoplasmic enzymes or localized in the nucleus, often as components of enzyme complexes. In many instances, these protein kinases are an essential element of enzyme and structural protein complexes that determine where and when a cellular process occurs within a cell.

Protein Tyrosine Kinases. Protein tyrosine kinases (PTKs) are enzymes which catalyse the phosphorylation of specific tyrosine residues in cellular proteins. This post-translational modification of these substrate proteins, often enzymes themselves, acts as a molecular switch regulating cell proliferation, activation or differentiation (for review, see Schlessinger and Ulrich, 1992, *Neuron* 9:383-391). Aberrant or excessive PTK activity has been observed in many disease states including benign and malignant proliferative disorders as well as diseases resulting from inappropriate activation of the immune system (e.g., autoimmune disorders), allograft rejection, and graft vs. host disease. In addition, endothelial-cell specific receptor PTKs such as KDR and Tie-2 mediate the angiogenic process, and are thus involved in supporting the progression of cancers and other diseases involving inappropriate vascularization (e.g., diabetic retinopathy, choroidal neovascularization due to age-related macular degeneration, psoriasis, rheumatoid arthritis, retinopathy of prematurity, infantile hemangiomas, psoriasis and atherosclerosis.

Tyrosine kinases can be of the receptor-type (having extracellular, transmembrane and intracellular domains) or the non-receptor type (being wholly intracellular).

Receptor Tyrosine Kinases (RTKs). The RTKs comprise a large family of transmembrane receptors with diverse biological activities. At present, at least nineteen (19) distinct RTK subfamilies have been identified. The receptor tyrosine kinase (RTK) family includes receptors that are crucial for the growth and differentiation of a variety of cell types (Yarden and Ullrich, *Ann. Rev. Biochem.*

57:433-478, 1988; Ullrich and Schlessinger, *Cell* 61:243-254, 1990). The intrinsic function of RTKs is activated upon ligand binding, which results in phosphorylation of the receptor and multiple cellular substrates, and subsequently in a variety of cellular responses (Ullrich & Schlessinger, 1990, *Cell* 61:203-212). Thus, receptor tyrosine kinase mediated signal transduction is initiated by extracellular interaction with a specific growth factor (ligand), typically followed by receptor dimerization, stimulation of the intrinsic protein tyrosine kinase activity and receptor trans-phosphorylation. Binding sites are thereby created for intracellular signal transduction molecules and lead to the formation of complexes with a spectrum of cytoplasmic signaling molecules that facilitate the appropriate cellular response. (e.g., cell division, differentiation, metabolic effects, changes in the extracellular microenvironment) see Schlessinger and Ullrich, 1992, *Neuron* 9:1-20.

Proteins with SH2 (src homology -2) or phosphotyrosine binding (PTB) domains bind activated tyrosine kinase receptors and their substrates with high affinity to propagate signals into cell. Both of the domains recognize phosphotyrosine. (Fantl *et al.*, 1992, *Cell* 69:413-423; Songyang *et al.*, 1994, *Mol. Cell. Biol.* 14:2777-2785; Songyang *et al.*, 1993, *Cell* 72:767-778; and Koch *et al.*, 1991, *Science* 252:668-678; Shoelson, *Curr. Opin. Chem. Biol.* (1997), 1(2), 227-234; Cowburn, *Curr. Opin. Struct. Biol.* (1997), 7(6), 835-838). Several intracellular substrate proteins that associate with receptor tyrosine kinases (RTKs) have been identified. They may be divided into two principal groups: (1) substrates which have a catalytic domain; and (2) substrates which lack such a domain but serve as adapters and associate with catalytically active molecules (Songyang *et al.*, 1993, *Cell* 72:767-778). The specificity of the interactions between receptors or proteins and SH2 or PTB domains of their substrates is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. For example, differences in the binding affinities between SH2 domains and the amino acid sequences surrounding the phosphotyrosine residues on particular receptors correlate with the observed differences in their substrate phosphorylation profiles (Songyang *et al.*, 1993, *Cell* 72:767-778). Observations suggest that the function of each receptor tyrosine kinase is determined not only by its pattern of expression and ligand availability but also by the array of

downstream signal transduction pathways that are activated by a particular receptor as well as the timing and duration of those stimuli. Thus, phosphorylation provides an important regulatory step which determines the selectivity of signaling pathways recruited by specific growth factor receptors, as well as differentiation factor receptors.

Several receptor tyrosine kinases such as FGFR-1, PDGFR, TIE-2 and c-Met, and growth factors that bind thereto, have been suggested to play a role in angiogenesis, although some may promote angiogenesis indirectly (Mustonen and Alitalo, *J. Cell Biol.* 129:895-898, 1995).

Tie-2 (TEK) is a member of a recently discovered family of endothelial cell specific receptor tyrosine kinases which is involved in critical angiogenic processes, such as vessel branching, sprouting, remodeling, maturation and stability. Tie-2 is the first mammalian receptor tyrosine kinase for which both agonist ligand(s) (e.g., Angiopoietin1 ("Ang1"), which stimulates receptor autophosphorylation and signal transduction), and antagonist ligand(s) (e.g., Angiopoietin2 ("Ang2")), have been identified. Knock-out and transgenic manipulation of the expression of Tie-2 and its ligands indicates tight spatial and temporal control of Tie-2 signaling is essential for the proper development of new vasculature. The current model suggests that stimulation of Tie-2 kinase by the Ang1 ligand is directly involved in the branching, sprouting and outgrowth of new vessels, and recruitment and interaction of periendothelial support cells important in maintaining vessel integrity and inducing quiescence. The absence of Ang1 stimulation of Tie-2 or the inhibition of Tie-2 autophosphorylation by Ang2, which is produced at high levels at sites of vascular regression, may cause a loss in vascular structure and matrix contacts resulting in endothelial cell death, especially in the absence of growth/survival stimuli. The situation is however more complex, since at least two additional Tie-2 ligands (Ang3 and Ang4) have recently been reported, and the capacity for heterooligomerization of the various agonistic and antagonistic angiopoietins, thereby modifying their activity, has been demonstrated. Targeting Tie-2 ligand-receptor interactions as an antiangiogenic therapeutic approach is thus less favored and a kinase inhibitory strategy preferred.

The soluble extracellular domain of Tie-2 ("ExTek") can act to disrupt the establishment of tumor vasculature in a breast tumor xenograft and lung metastasis models and in tumor-cell mediated ocular neovasculatization. By adenoviral infection, the *in vivo* production of mg/ml levels ExTek in rodents may be achieved for 7-10 days with no adverse side effects. These results suggest that disruption of Tie-2 signaling pathways in normal healthy animals may be well tolerated. These Tie-2 inhibitory responses to ExTek may be a consequence of sequestration of ligand(s) and/or generation of a nonproductive heterodimer with full-length Tie-2.

Recently, significant upregulation of Tie-2 expression has been found within the vascular synovial pannus of arthritic joints of humans, consistent with a role in the inappropriate neovascularization. This finding suggests that Tie-2 plays a role in the progression of rheumatoid arthritis. Point mutations producing constitutively activated forms of Tie-2 have been identified in association with human venous malformation disorders. Tie-2 inhibitors are, therefore, useful in treating such disorders, and in other situations of inappropriate neovascularization.

The Examples herein describe the preparation and crystallization of polypeptides comprising the catalytic domain of human Tie-2. As used herein, the term "catalytic domain" refers to a specific module common to all kinases which bind ATP, such as the tyrosyl binding site, the site where ATP binds including the metal-ion binding region, and the site where the phosphoryl transfer occurs. For Tie-2, the catalytic domain is defined by amino acid residues from about residue 828 to about residue 985 of SEQ ID NO: 1, with residues 828-840, 853-855, 872, 873, 876, 879, 880, 885-888, 900, 902-909, 912, 954, 955, 960, 964, 968-971, and 980-985 included in the catalytic domain.

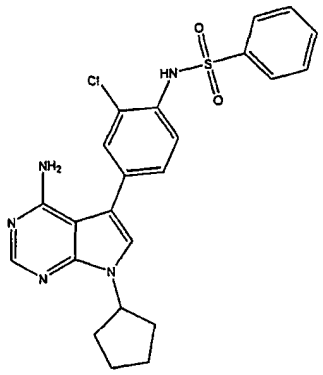
The amino acid sequences of native human Tie-2 (SEQ ID NO: 1) is taken as defined in SWISS-PROT (Ziegler, et al. *Oncogene,* **8**:663 (1993)). As described in the Examples, certain of these crystals were examined by x-ray crystallography and atomic coordinates for the peptide were obtained. In certain cases, the polypeptide was unligated, that is, not complexed with a ligand. In other cases, the polypeptide was complexed with a ligand and the atomic coordinates of the ligand bound to the Tie-2 catalytic domain were also obtained.

Tie-2 is subject to autophosphorylation and transphosphorylation by other proteins. Phosphorylation state is a particularly important posttranslational modification to consider. A wild-type construct (i.e., without the D964N mutation) having residues 802-1124 of SEQ ID NO 1 was isolated from an expression system as a singly- or a multiply-phosphorylated species. One singly-phosphorylated species has its phosphate on either Y897 or Y899. In multiply phosphorylated species, phosphorylation can be on combinations of many Y residues on the protein. A diphosphorylated species crystallized in the space group P2(1)2(1)2(1) with the unit cell dimensions of a = 54.320 Å, b = 75.872 Å, c = 78.143 Å, and $\alpha = \beta = \gamma = 90.0°$. The term "space group" is a term of art which refers to the collection of symmetry elements of the unit cell of a crystal. Other phosphorylation sites are described in Jones, N., *et al.*, *J. Biol. Chem.* (1999), *274*(43):30896.

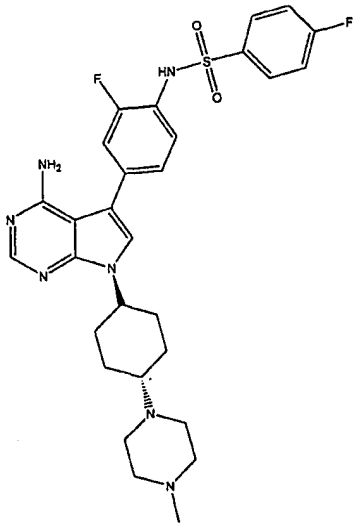
A catalytically inactive mutant of human Tie-2 (SEQ ID NO 2) was also crystallized. The catalytically inactive mutant had the same sequence as residues 802 to 1124 of human Tie-2 except that residue 964 which is aspartic acid in wild type human Tie-2 was replaced with asparagine. This substitution rendered the mutant catalytically inactive. SEQ ID NO 2 crystallized in the space group C222(1) which had the unit cell dimensions a = 75.195 Å, b = 116.287 Å, c = 95.060 Å, and $\alpha = \beta = \gamma = 90.0°$

The atomic coordinates for four crystals of Tie-2/ligand complexes examined by x-ray crystallography are presented in Figs. 3A-3OO, 4A-4OO, 5A-5RR and 6A-6NN. The term "atomic coordinates" (or "structural coordinates") refers to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of x-rays by atoms (scattering centers) of a crystalline polypeptide comprising a Tie-2 catalytic domain molecule. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal. Atomic coordinates can be transformed as is known in the art to different coordinate systems without affecting the relative positions of the atoms.

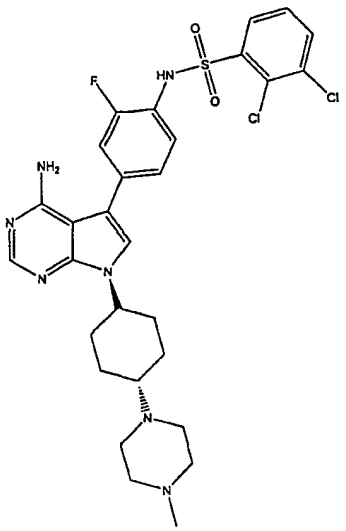
In particular, four high resolution crystal structures were obtained for SEQ ID NO 2) complexed with one of four different inhibitors shown below:



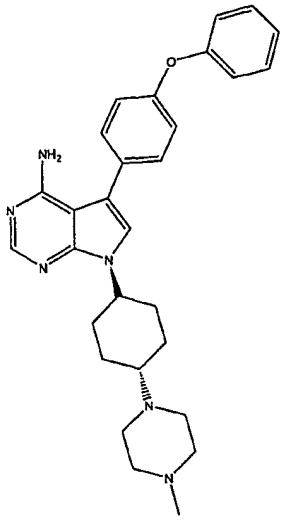
Inhibitor I



Inhibitor II



Inhibitor III



Inhibitor IV

The results of the x-ray crystal structure determination for SEQ ID NO 2, the catalytic domain of human Tie-2, showed the following features:

The overall structure adopted a recognizable kinase fold with an N-terminal lobe and a somewhat larger C-terminal lobe. ATP binding was at the interface of the two lobes with inhibitors also binding in this region. The major secondary structural elements of the N-terminal lobe were a five strand beta sheet and a long alpha helix. The C-terminal lobe was primarily a bundle of alpha helices with a short, two-strand beta sheet near the interface with the N-terminal lobe. Fig. 7 shows a prototypical receptor tyrosine kinase, insulin receptor kinase which highlights the structural features associated with known kinases. The structure of the catalytic domain of Tie-2, shown in Fig. 9 has similar features to this

The hinge region connects the N-terminal and C-terminal lobes. The portion of the hinge which forms part of the ATP/inhibitor binding region presents several hydrogen bonding partners. The carbonyl oxygen atoms of E903, A905 and P906 and the backbone amide protons of A905, H907 and G908 were presented into the pocket. The sidechains of L900, I902, Y904 and A905 helped to define the size, shape and nature of the binding pocket.

The purine core binding region was the region where the N-terminal and C-terminal lobes of the protein cooperate to form a flat, predominantly hydrophobic binding region which is the traditional location for the purine ring of ATP in other kinase structures. The residues which contribute to this region included: I830, A853, V838, I886, L971 and A981. Sidechains of residues in the hinge region, I902, Y904 and A905 also contributed hydrophobic character to this region. The carbonyl oxygen of I830 and the amide proton of V838 also presented an interaction site within this region.

By analogy to known kinase structures, the ribose ring of ATP would traditionally occupy an area between G831 in the N-terminal lobe and N909 in the C-terminal lobe called the extended sugar pocket. The backbone amide protons of G831, E832 and N909, the carbonyl oxygen of R968 and the sidechains of E832, N909 and D912 presented hydrogen bond partners.

By anaology to known kinase structures, the γ-phosphate of ATP would occupy an area around the sidechains of residues D964 (N964 in the catalytically inactive mutant, SEQ ID NO 2). The sidechain of R968 also contributes to this

region. The predominant available interaction type was hydrogen bonding, with quite complex coordination possible.

The nucleotide binding loop, or glycine-rich loop, was a flap like loop in the N-terminal lobe which covered the front portion of the ATP binding region. Residues not already described in other binding areas include D828, V829, G833, N834, F835, G836, Q837, L839, and K840. Residues I830, G831, E832 and V838 were also part of this structural element, but have already been included in other binding regions described above. This loop is usually considered to be very flexible and is capable of altering the shape and size of the ATP binding region. Carbonyl oxygen atoms, N834 sidechain atoms and backbone amide protons of G833, N834 and F835 were potentially available for hydrogen bonding. The sidechain atoms of D828 and K840 were available for ionic/hydrogen bonding interactions. The sidechain atoms of V829, I830, F835 and L839 can contribute to hydrophobic interactions.

The early activation loop was a long flexible loop containing at least one residue, the phosphorylation of which, is generally believed to determine the activation state of the protein. The loop begins in the ATP binding site and ends in the C-terminal lobe in the area which most likely corresponds to substrate binding. Residues F983, G984, and L985 form part of the ATP binding site and were also on the N-terminal side of the activation loop. The carboxyl oxygen and amide protons of F983 and G984 and the amide proton of L985 were available for hydrogen bonding and the sidechains of F983 and L985 can contribute to hydrophobic interactions.

K855, by homology to known kinases, is part of the catalytic mechanism of the kinase. The amino group can participate in ionic or hydrogen bond interactions and the methylene groups can contribute to hydrophobic interactions. The sidechain is very mobile.

The distal hydrophobic pocket is is characterized by a buried hydrophobic cavity. This portion of the ATP binding region is not occupied by any ATP atoms in known kinase structures. Residues which contribute to this pocket include L873, L876, L879, I885, L888, Y954, L955, F960 and I980. I886, A981 and F983 from regions already described also contribute hydrophobic interactions to this region. In addition, there was a number of backbone hydrogen bond partners available in this

area. These partners included the carbonyl oxygen atoms of I886, L879, and G880. With the apparent disruption of the alpha-C helix, carbonyl oxygen atoms of E872, L873 and L876 may also be available. The backbone amide proton of residues, I886 and L888 were also available in this region.

Several residues contributed to the ATP/inhibitor binding site but do not seem to be part of definable subregion. These residues are I854, E872, N887, I970 and I980. E872 often forms an ionic interaction with the catalytic lysine in known kinase structures. N887 may contribute to the distal hydrophobic pocket. The sidechains of I854, and I970 face away from the ATP pocket, however carbonyl oxygen atoms from these residues as well as I980 were presented towards the binding region.

The structure of the SEQ ID NO 2/inhibitor I complex had the following features:

Final resolution of the structure was 2.8 Å in space group C2221, with final coordinates determined for backbone atoms of residues 818-857, 864-995, 1001-1116.

The pyrrolopyrimidine ring of inhibitor I formed hydrogen bonds to residues in the hinge region and interacts with purine core region. The core of the inhibitor presented a hydrogen bond donor in the form of the amino proton of the 4-NH_2 substituent to the carbonyl oxygen of E903. Atom N3 of the pyrimidine ring accepted a hydrogen bond from the backbone N-H of A905. The ring system of the core presented a planar face to residues of both the C-terminal and N-terminal lobes. The residues in these areas present a hydrophobic surface which "sandwiches" the planar core of the inhibitor. Residues involved in this hydrophobic sandwich region include I830, V838, I86, I902 and L971. Atoms N1 and N7 of the inhibitor core faced the solvent exposed mouth of the binding pocket. Atom C6 of the inhibitor faced the long axis of the nucleotide binding loop of the N-terminal lobe of the protein.

The N7 cyclopentane ring of Inhibitor I was directed towards solvent but was still within the protein cavity. This region was described above as the extended sugar pocket. This region was characterized by hydrophobic interactions with primarily I830 and L971. Methylene groups of E832 may also contribute in this fashion.

The phenyl ring attached to C5 of the pyrrolopyrimidine ring was in a predominantly hydrophobic area, generated by residues from the purine core region,

the distal hydrophobic pocket and methylene groups from the catalytic lysine, K855. The hydrophobic contacts were with residues V838, I886, I902, L971 and A981. Lysine 855 was highly mobile, so it is also possible that the chlorine atom meta to the pyrrolopyrimidine ring was receiving a hydrogen bond.

The sulfonamide linker made a clear hydrogen bond with an amide proton of D982 and may also make a hydrogen bond to the amide proton of F983.

The terminal phenyl ring was located in the distal hydrophobic pocket. Primary contacts were with L876, I886, L888 and F983.

The structure of the SEQ ID NO 2/inhibitor II, SEQ ID NO 2/inhibitor III and SEQ ID NO 2/inhibitor IV complexes had the following features:

Residues 818-857, 864-995, 1001-1116 have been modeled into the solved structure. A space group P42212 was observed. The overall fold is still a standard kinase catalytic domain fold and the binding regions described above for SEQ ID NO 2/inhibitor I still pertain.

The pyrrolopyrimidine core, B-ring, linker and C-ring of inhibitor II in the SEQ ID NO 2/inhibitor II complex was bound the same way as inhibitor I. In addition, the N-7 cyclohexyl N-methyl piperazinyl group occupied the extended sugar pocket and made a strong ionic interaction with D912.

The pyrrolopyrimidine of inhibitor III binds was bound the same way in the SEQ ID NO 2/inhibitor III complex as inhibitor I. The N-7 cyclohexyl N-methy piperazinyl group occupied the extended sugar pocket and made a strong ionic interaction with D912 as in the SEQ ID NO 2/inhibitor II complex. The B-ring was bound in a similar fashion to inhibitor I, however, the hydrogen bond between halogens, fluorine in this case, and K855 was more clear. The sulfonyl oxygens of the sulfonamide linker made two clear hydrogen bonds to backbone amide protons of D983 and F983. The C-ring occupied the distal hydrophobic pocket with main interactions coming from L876, I886, L888, L900, I902 and F983.

The pyrrolopyrimidine core of inhibitor IV in the SEQ ID NO 2/inhibitor IV complex was bound the same way as inhibitor I. The N-7 cyclohexyl N-methyl piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912 as in SEQ ID NO 2/inhibitor II. The B-ring binds in a similar

fashion to inhibitor I, however there is no halogen atom to act as a potential hydrogen bond partner in inhibitor IV. The oxygen atom of the linker accepted a hydrogen bond from the catalytic lysine, K855. The C-ring of inhibitor IV occupied the distal hydrophobic pocket with main interactions coming from L876, I886, I902 and F983.

Analysis of the three dimensional structure of the Tie-2 catalytic domain has indicated the presence of a number of subsites, each of which includes molecular functional groups capable of interacting with complementary moieties of an inhibitor. Subsites 1 through 9 of the Tie-2 catalytic domain are defined below. A summary of the properties of the chemical moieties present at each subsite is given below. Subsites are characterized below according to the properties of chemical moieties with which they are complementary, or with which they can interact. Such moieties can include hydrogen bond acceptors, such as hydroxyl, amino, ether, thioether, carboxyl, P=O, and carbonyl groups, halogen atoms, such as fluorine, chlorine, bromine and iodine atoms; and other groups including a heteroatom having at least one lone pair of electrons, such as groups containing trivalent phosphorous, di- and tetravalent sulfur, oxygen and nitrogen atoms; hydrogen bond donors, such as hydroxyl, thiol, an amide proton, amine protons, carboxylic acid groups and any of the groups listed under hydrogen atom acceptors to which a hydrogen atom is bonded; hydrophobic groups, such as linear, branched or cyclic alkyl, ether or thioalkyl groups; linear, branched or cyclic alkenyl groups; linear, branched or cyclic alkynyl groups; aryl groups, such as mono- and polycyclic aromatic hydrocarbyl groups and mono- and polycyclic heterocyclic or heteroaryl groups; positively charged groups, such as primary, secondary, tertiary and quaternary ammonium groups, imidazolium and other protonated heteroalkyl and heteroaryl moieties, substituted and unsubstituted guanidinium groups, sulfonium groups and phosphonium groups; and negatively charged groups, such as carboxylate, phenolate, thiolate, sulfonamide, sulfamate, boronate, vanadate, sulfonate, sulfinate, phosphinate, tetrazolate and other heteroaryl anions, heterocyclic N-oxides, and phosphonate groups. A given chemical moiety can contain one or more of these groups.

Subsite 1: Hinge Region

Hydrogen Acceptors: The the backbone carbonyl oxygen of residues E903, A905 and P906 present proton acceptors.

Hydrogen Donors: The backbone amide protons of residues A905, H907 and G908 present proton donors.

Hydrophobic Groups: The sidechains of L900, I902, Y904 and A905 present hydrophobic groups.

Subsite 2: The Purine Core Binding Region

Hydrophobic Groups: Residues I830, A853, V838, I886, L971, A981 and the sidechains of residues I902, Y904, and A905 present hydrophobic groups.

Hydrogen Acceptors: The carbonyl oxygen of I830 presents a proton acceptor.

Hydrogen Donors: The amide proton of V838 presents a proton donor.

Subsite 3: The Extended Sugar Pocket

Hydrogen Acceptors: The backbone carbonyl oxygen of R968 and the sidechain carbonyl oxygen of E832, N909 and D912 present proton acceptors.

Hydrogen Donors: The backbone amide protons of G831, E832 and N909 present proton donors.

Subsite 4: The Extended γ-Phosphate Region

Hydrogen Bonding Groups: Residues D964 (N964 in the catalytically inactive mutant), N969 and D982 present both proton donor and proton acceptor groups.

Subsite 5: The Nucleotide binding Loop

Hydrogen Acceptors: The carbonyl oxygen of the sidechain of residue N834 presents a proton acceptor.

Hydrogen Donors: The backbone amide protons of residues G833, N834 and F835 present proton donors.

Positively Charged Group: The sidechain of K840 presents a positively charged site.

Negatively Charged Group: The sidechain of D828 presents a negatively charged site.

Hydrophobic Groups: The sidechains of V829, I830, F835 and L839 present hydrophobic groups.

Subsite 6: The Early Activation Loop

Hydrogen Acceptors: The backbone carbonyl oxygens of residues F983 and G984 presents a proton acceptor.

Hydrogen Donors: The backbone amide protons of residues F983, G984 and L985 present proton donors.

Hydrophobic Groups: The sidechains of F983 and L985 present hydrophobic groups.

Subsite 7: The Catalytic Lysine

Positively Charged Group: The sidechain of K855 presents a positively charged site.

Hydrophobic Group: The methylene groups of the sidechain of K855 presents a hydrophobic group.

Subsite 8: The Distal Hydrophobic Pocket

Hydrophobic Groups: Residues L873, L876, L879, I885, L888, Y954, L955, F960, I980, I886, A981 and F983 present hydrophobic groups.

Hydrogen Acceptors: The backbone carbonyl oxygens of residues I886, L879, G880, E872, L873 and L876 present proton acceptors.

Hydrogen Donors: The backbone amide protons of residues I886 and L888 present proton donors.

Subsite 9: Miscellaneous interaction sites which contribute to the ATP binding site.

Hydrogen Acceptors: The backbone carbonyl oxygens of residues I854, I970 and I980 present proton acceptors in the ATP binding region.

Negatively Charged Groups: E872 presents a negatively charged group which often forms an ionic bond with the catalytic lysine residue K855.

Fig. 9 provides a model of the catalytic domain of Tie-2 bound to inhibitor I. Subsites 1-9 of the catalytic domain are each depicted in a different color as follows:

the hinge region (dark blue), the purine core (light blue), the extended sugar pocket (light purple), the γ-phosphate region (dark yellow), the nucleotide binding loop (red), the early activation loop (dark green), the catalytic lysine (light green), the distal hydrophobic pocket (dark purple), and miscellaneous interaction sites (brown). The inhibitor is depicted in light yellow.

In one embodiment, the present invention provides polypeptides comprising the catalytic domain of Tie-2, crystalline forms of these polypeptides, optionally complexed with a ligand, and the three dimensional structure of the polypeptides, including the three dimensional structure of the Tie-2 catalytic domain. In general, these three dimensional structures are defined by atomic coordinates derived from x-ray crystallographic studies of the polypeptides. The catalytic domain can be unphosphorylated, monophosphorylated or multiply phosphorylated. Phosphorylization typically occurs at tyrosine residues. One monophosphorylated species has a phosphate group on Y897 or Y899.

The polypeptides can include the catalytic domain of Tie-2 from any species, such as a yeast or other unicellular organism, an invertebrate or a vertebrate. Preferably, the polypeptide includes the catalytic domain of a mammalian Tie-2, such as murine Tie-2. More preferably, the polypeptide includes the catalytic domain of human Tie-2. The polypeptides of the invention also includes polypeptides comprising single nucleotide polymorphisms of the catalytic domain of human Tie-2 or murine Tie-2. In one embodiment, the polypeptides of the invention, and crystalline forms thereof, include a sequence which has at least 80% identity to the catalytic domain of human Tie-2 or murine Tie-2.

To determine the percent identity of two amino acid sequences, the sequences are aligned for optimal comparison purposes (*e.g.*, gaps can be introduced in one or both of a first and a second amino acid or nucleic acid sequence for optimal alignment, and non-homologous (dissimilar) sequences can be disregarded for comparison purposes). In a preferred embodiment, the length of a first sequence aligned for comparison purposes is at least 30%, preferably at least 40%, more preferably at least 50%, even more preferably at least 60%, and even more preferably at least 70%, 80%, or 90% of the length of the second sequence. The amino acid

residues at corresponding amino acid positions are then compared. When a position in the first sequence is occupied by the same amino acid residue as the corresponding position in the second sequence, then the molecules are identical at that position. The percent identity between the two sequences is a function of the number of identical positions shared by the sequences, taking into account the number of gaps, and the length of each gap, which need to be introduced for optimal alignment of the two sequences.

The invention also encompasses polypeptides having a lower degree of identity but having sufficient homology so as to perform one or more of the same functions performed by Tie-2 polypeptides described herein by amino acid sequence. Homology for a polypeptide is determined by conservative amino acid substitution. Such substitutions are those that substitute a given amino acid in a polypeptide by another amino acid of like characteristics. Conservative substitutions are likely to be phenotypically silent. Typically seen as conservative substitutions are the replacements, one for another, for example, among the aliphatic amino acids Ala, Val, Leu, and Ile; interchange of the hydroxyl residues Ser and Thr, exchange of the acidic residues Asp and Glu, substitution between the amide residues Asn and Gln, exchange of the basic residues Lys and Arg or replacements among the aromatic residues Phe, Tyr and Trp. Guidance concerning which amino acid changes are likely to be phenotypically silent is found in Bowie *et al., Science 247*:1306-1310 (1990).

The comparison of sequences and determination of percent identity and homology between two sequences can be accomplished using a mathematical algorithm. (*Computational Molecular Biology*, Lesk, A.M.,ed., Oxford University Press, New York, 1988; *Biocomputing: Informatics and Genome Projects,* Smith, D.W., ed., Academic Press, New York, 1993; *Computer Analysis of Sequence Data, Part 1,* Griffin, A.M., and Griffin, H.G., eds., Humana Press, New Jersey, 1994; *Sequence Analysis in Molecular Biology,* von Heinje, G., Academic Press, 1987; and *Sequence Analysis Primer*, Gribskov, M. and Devereaux, J., eds., M. Stockton Press, New York, 1991). In a preferred embodiment, the percent identity between two amino acid sequences is determined using the Needleman and Wunsch (*J. Mol. Biol.* (48):444-453 (1970)) algorithm which has been incorporated into the GAP program in

the GCG software package (available on March 29, 2000 at http://www.gcg.com), using either a Blossom 62 matrix or a PAM250 matrix, and a gap weight of, for example, 16, 14, 12, 10, 8, 6, or 4 and a length weight of, for example, 1, 2, 3, 4, 5, or 6. In yet another preferred embodiment, the percent identity between two nucleotide sequences is determined using the GAP program in the GCG software package (Devereux, J., *et al.*, *Nucleic Acids Res. 12(1)*:387 (1984)) (available on March 29, 2000 at http://www.gcg.com), using a NWSgapdna.CMP matrix and a gap weight of, for example, 40, 50, 60, 70, or 80 and a length weight of, for example, 1, 2, 3, 4, 5, or 6. In another embodiment, the percent identity between two amino acid or nucleotide sequences is determined using the algorithm of E. Meyers and W. Miller (*CABIOS, 4*:11-17 (1989)) which has been incorporated into the ALIGN program (version 2.0), using, for example, a PAM120 weight residue table, a gap length penalty of 12 and a gap penalty of 4.

The protein sequences of the present invention, for example, amino acids 802-1124 of human Tie-2 (SEQ ID NO 1), can further be used as a "query sequence" to perform a search against databases to, for example, identify other family members or related sequences. Such searches can be performed using the NBLAST and XBLAST programs (version 2.0) of Altschul, *et al.* (*J. Mol. Biol. 215*:403-10 (1990)). BLAST protein searches can be performed with the XBLAST program, for example, score = 50, word length = 3, to obtain amino acid sequences homologous to the proteins of the invention. To obtain gapped alignments for comparison purposes, gapped BLAST can be utilized as described in Altschul *et al.*, *(Nucleic Acids Res. 25*(17):3389-3402 (1997)). When utilizing BLAST and gapped BLAST programs, the default parameters of the respective programs (*e.g.*, XBLAST and NBLAST) can be used as given on March 29, 2000 at http://www.ncbi.nlm.nih.gov.

Homology for amino acid sequences can be defined in terms of the parameters set by the Advanced Blast search available from NCBI (the National Center for Biotechnology Information; see, for Advanced BLAST , www.ncbi.nlm.nih.gov/cgi-bin/BLAST/nph-newblast?Jform=1 (on March 29, 2000)). These default parameters, recommended for a query molecule of length greater than 85 amino acid residues or nucleotides have been set as follows: gap existence cost, 11, per residue gap cost, 1;

lambda ratio, 0.85. Further explanation of version 2.0 of BLAST can be found on related website pages and in Altschul, S.F. *et al., Nucleic Acids Res. 25*:3389-3402 (1997).

In one embodiment, the polypeptide includes amino acids 802 to 1124 of SEQ ID NO: 1. Polypeptides can also have amino acids 792 to 1124, 782 to 1124, 772 to 1124, 812 to 1124, 822 to 1124, 832 to 1124, 802 to 1114, 802 to 1104, or 802 to 1094 of SEQ ID NO 1. In another embodiment, the polypeptide can be a catalytically inactive mutant of Tie-2, such as SEQ ID NO 2, wherein the asparagine amino acid at 964 is replaced with an aspartic acid amino acid (designated D964N mutant). Other catalytically inactive mutants include substitution of the asparagine amino acid at 964 with alanine, serine, threonine, or glycine.

In another embodiment, the catalytic domain which is crystallized can have deletions of amino acids from the native sequence. For example, a polypeptide which is suitable for crystallization can include amino acids 802 to 918 of SEQ ID NO 1 fused to amino acids 934 to 1124 of SEQ ID NO 1 or other related "kinase-insert domain" deletions.

The crystalline polypeptide, preferably, further includes a ligand bound to the Tie-2 catalytic domain. The ligand is, preferably, a small (less than about 1500 molecular weight) organic molecule, for example, inhibitor I, II, III, or IV.

In one embodiment, the invention relates to a method of determining the three dimensional structure of a first polypeptide comprising the catalytic domain of a Tie-2 protein. The method includes the steps of (1) obtaining a crystal comprising the first polypeptide; (2) obtaining x-ray diffraction data for said crystal; and (3) using the x-ray diffraction data and the atomic coordinates of a second polypeptide comprising the catalytic domain of a Tie-2 protein to solve the crystal structure of the first polypeptide, thereby determining the three dimensional structure of the first polypeptide. The second polypeptide can include the same Tie-2 catalytic domain as the first polypeptide, or a different Tie-2 catalytic domain. Either or both of the first and second polypeptides can, optionally, be complexed with a ligand. That is, the crystal of the first polypeptide can comprise a complex of the first polypeptide with a ligand. The atomic coordinates of the second polypeptide can, optionally, include the

atomic coordinates of a ligand molecule bound to the second polypeptide. The atomic coordinates of the second polypeptide, generally, have been previously obtained, for example, by x-ray crystallographic analysis of a crystal comprising the second polypeptide or a complex of the second polypeptide with a ligand. The atomic coordinates of the second polypeptide can be used to solve the crystal structure using methods known in the art, for example, molecular replacement or isomorphous replacement. Preferably, the second polypeptide comprises the catalytic domain of a mammalin Tie-2, more preferably, human Tie-2. For example the atomic coordinates which can be used include the atomic coordinates presented herein, preferably the atomic coordinates presented in Figures 3-7.

The invention also provides a method of identifying a compound which is a potential inhibitor of Tie-2. The method comprises the steps of (1) obtaining a crystal of a polypeptide comprising the catalytic domain of Tie-2; (2) obtaining the atomic coordinates of the polypeptide by x-ray diffraction studies using said crystal; (3) using said atomic coordinates to define the catalytic domain of Tie-2; and (4) identifying a compound which fits the catalytic domain. The method can further include the steps of obtaining, for example, from a compound library, or synthesizing the compound identified in step 4, and assessing the ability of the identified compound to inhibit Tie-2 enzymatic activity.

The polypeptide preferably comprises the catalytic domain of a mammalian Tie-2. More preferably the polypeptide comprises the catalytic domain of human Tie-2. In a preferred embodiment, the polypeptide is a polypeptide of the present invention, as described above.

The polypeptide can be crystallized using methods known in the art, such as the methods described in the Examples, to afford polypeptide crystals which are suitable for x-ray diffraction studies. A crystalline polypeptide/ligand complex can be produced by soaking the resulting crystalline polypeptide in a solution including the ligand. Preferably, the ligand solution is in a solvent in which the polypeptide is insoluble.

The atomic coordinates of the polypeptide (and ligand) can be determined, for example, by x-ray crystallography using methods known in the art. The data obtained

from the crystallography can be used to generate atomic coordinates, for example, of the atoms of the polypeptide and ligand, if present. As is known in the art, solution and refinement of the x-ray crystal structure can result in the determination of coordinates for some or all of the non-hydrogen atoms. The atomic coordinates can be used, as is known in the art, to generate a three-dimensional structure of the Tie-2 catalytic domain. This structure can then be used to assess the ability of any given compound, preferably using computer-based methods, to fit into the catalytic domain.

A compound fits into the catalytic domain if it is of a suitable size and shape to physically reside in the catalytic domain, that is, if it has a shape which is complementary to the catalytic domain and can reside in the catalytic domain without significant unfavorable steric or van der Waals interactions. Preferably, the compound includes one or more functional groups and/or moieties which interact with one or more subsites within the catalytic domain. Computational methods for evaluating the ability of a compound to fit into the catalytic domain, as defined by the atomic coordinates of the polypeptide, are known in the art, and representative examples are provided below.

In another embodiment, the method of identifying a potential inhibitor of Tie-2 comprises the step of determining the ability of one or more functional groups and/or moieties of the compound, when present in the Tie-2 catalytic domain, to interact with one or more subsites of the Tie-2 catalytic domain. Preferably, the Tie-2 catalytic domain is defined by the atomic coordinates of a polypeptide comprising the Tie-2 catalytic domain. If the compound is able to interact with a preselected number or set of subsites, the compound is identified as a potential inhibitor of Tie-2.

A functional group or moiety of the compound is said to "interact" with a subsite of the Tie-2 catalytic domain if it participates in an energetically favorable, or stabilizing, interaction with one or more complementary moieties within the subsite. Two chemical moieties are "complementary" if they are capable, when suitably positioned, of participating in an attractive, or stabilizing, interaction, such as an electrostatic or van der Waals interaction. Typically, the attractive interaction is an ion-ion (or salt bridge), ion-dipole, dipole-dipole, hydrogen bond, pi-pi or hydrophobic interaction. For example, a negatively charged moiety and a positively

charged moiety are complementary because, if suitably positioned, they can form a salt bridge. Likewise, a hydrogen bond donor and a hydrogen bond acceptor are complementary if suitably positioned.

Typically, an assessment of interactions between the test compound and the Tie-2 catalytic domain may employ computer-based computational methods, such as those known in the art, in which possible interactions of a compound with the protein, as defined by atomic coordinates, are evaluated with respect to interaction strength by calculating the interaction energy upon binding the compound to the protein. Compounds which have calculated interaction energies within a preselected range or which otherwise, in the opinion of the computational chemist employing the method, have the greatest potential as Tie-2 inhibitors, can then be provided, for example, from a compound library or via synthesis, and assayed for the ability to inhibit Tie-2. The interaction energy for a given compound generally depends upon the ability of the compound to interact with one or more subsites within the protein catalytic domain.

In one embodiment, the atomic coordinates used in the method are the atomic coordinates set forth in Figs. 3A-3OO, 4A-4OO, 5A-5RR and 6A-6NN. It is to be understood that the coordinates set forth in Figs. 3-6 can be transformed, for example, into a different coordinate system, in ways known to those skilled in the art without substantially changing the three dimensional structure represented thereby.

In certain cases, a moiety of the compound can interact with a subsite via two or more individual interactions. A moiety of the compound and a subsite can interact if they have complementary properties and are positioned in sufficient proximity and in a suitable orientation for a stabilizing interaction to occur. The possible range of distances for the moiety of the compound and the subsite depends upon the distance dependence of the interaction, as is known in the art. For example, a hydrogen bond typically occurs when a hydrogen bond donor atom, which bears a hydrogen atom, and a hydrogen bond acceptor atom are separated by about 2.5 Å and about 3.5 Å. Hydrogen bonds are well known in the art (Pimentel *et al.*, *The Hydrogen Bond*, San Francisco: Freeman (1960)). Generally, the overall interaction, or binding, between the compound and the Tie-2 catalytic domain will depend upon the number and strength of these individual interactions.

The ability of a test compound to interact with one or more subsites of the catalytic domain of Tie-2 can be determined by computationally evaluating interactions between functional groups, or moieties, of the test compound and one or more amino acid side chains in a particular protein subsite, such as subsites 1 to 9 above. Typically, a compound which is capable of participating in stabilizing interactions with a preselected number of subsites, preferably without simultaneously participating in significant destabilizing interactions, is identified as a potential inhibitor of Tie-2. Such a compound will interact with one or more subsites, preferably with two or more subsites and, more preferably, with three or more subsites.

The invention further provides a method of designing a compound which is a potential inhibitor of Tie-2. The method includes the steps of (1) identifying one or more functional groups capable of interacting with one or more subsites of the Tie-2 catalytic domain; and (2) identifying a scaffold which presents the functional group or functional groups identified in step 1 in a suitable orientation for interacting with one or more subsites of the Tie-2 catalytic domain. The compound which results from attachment of the identified functional groups or moieties to the identified scaffold is a potential inhibitor of Tie-2. The Tie-2 catalytic domain is, generally, defined by the conserved homolohous sequence when compared to other known tyrosine kinases, for example, the atomic coordinates set forth in Figs. 3A-3OO, 4A-4OO, 5A-5RR and 6A-6NN.

Suitable methods, as are known in the art, can be used to identify chemical moieties, fragments or functional groups which are capable of interacting favorably with a particular subsite or set of subsites. These methods include, but are not limited to: interactive molecular graphics; molecular mechanics; conformational analysis; energy evaluation; docking; database searching; pharmacophore modeling; de novo design and property estimation. These methods can also be employed to assemble chemical moieties, fragments or functional groups into a single inhibitor molecule. These same methods can also be used to determine whether a given chemical moiety, fragment or functional group is able to interact favorably with a particular subsite or set of subsites.

In one embodiment, the design of potential human Tie-2 inhibitors begins from the general perspective of three-dimensional shape and electrostatic complementarity for the catalytic domain, encompassing subsites 1-9, and subsequently, interactive molecular modeling techniques can be applied by one skilled in the art to visually inspect the quality of the fit of a candidate inhibitor modeled into the binding site. Suitable visualization programs include INSIGHTII (Molecular Simulations Inc., San Diego, CA), QUANTA (Molecular Simulations Inc., San Diego, CA), SYBYL (Tripos Inc., St Louis, MO), RASMOL (Roger Sayle *et al.*, *Trends Biochem. Sci.* **20**: 374-376 (1995)), GRASP (Nicholls *et al.*, *Proteins* **11**: 281-289 (1991)), and MIDAS (Ferrin *et al.*, *J. Mol. Graphics* **6**:13-27 (1988)).

A further embodiment of the present invention utilizes a database searching program which is capable of scanning a database of small molecules of known three-dimensional structure for candidates which fit into the target protein site. Suitable software programs include CATALYST (Molecular Simulations Inc., San Diego, CA), UNITY (Tripos Inc., St Louis, MO), FLEXX (Rarey et al., *J. Mol. Biol.* **261**: 470-489 (1996)), CHEM-3DBS (Oxford Molecular Group, Oxford, UK), DOCK (Kuntz *et al.*, *J. Mol. Biol* **161**: 269-288 (1982)), and MACCS-3D (MDL Information Systems Inc., San Leandro, CA). It is not expected that the molecules found in the search will necessarily be leads themselves, since a complete evaluation of all interactions will necessarily be made during the initial search. Rather, it is anticipated that such candidates might act as the framework for further design, providing molecular skeletons to which appropriate atomic replacements can be made. Of course, the chemical complimentary of these molecules can be evaluated, but it is expected that the scaffold, functional groups, linkers and/or monomers may be changed to maximize the electrostatic, hydrogen bonding, and hydrophobic interactions with the enzyme. Goodford (Goodford *J Med Chem* **28**:849-857 (1985)) has produced a computer program, GRID, which seeks to determine regions of high affinity for different chemical groups (termed probes) on the molecular surface of the binding site. GRID hence provides a tool for suggesting modifications to known ligands that might enhance binding.

A range of factors, including electrostatic interactions, hydrogen bonding, hydrophobic interactions, desolvation effects, conformational strain or mobility, chelation and cooperative interaction and motions of ligand and enzyme, all influence the binding effect and should be taken into account in attempts to design bioactive inhibitors.

Yet another embodiment of a computer-assisted molecular design method for identifying inhibitors comprises searching for fragments which fit into a binding region subsite and link to a predefined scaffold. The scaffold itself may be identified in such a manner. Programs suitable for the searching of such functional groups and monomers include LUDI (Boehm, *J Comp. Aid. Mol. Des.* **6**:61-78 (1992)), CAVEAT (Bartlett *et al.* in "Molecular Recognition in Chemical and Biological Problems", special publication of *The Royal Chem. Soc.*, **78**:182-196 (1989)) and MCSS (Miranker *et al. Proteins* **11**: 29-34 (1991)).

Yet another embodiment of a computer-assisted molecular design method for identifying inhibitors of the subject phosphatase comprises the *de novo* synthesis of potential inhibitors by algorithmic connection of small molecular fragments that will exhibit the desired structural and electrostatic complementarity with the active site of the enzyme. The methodology employs a large template set of small molecules with are iteratively pieced together in a model of the Tie-2 active site. Programs suitable for this task include GROW (Moon *et al. Proteins* **11**:314-328 (1991)) and SPROUT (Gillet *et al. J Comp. Aid. Mol. Des.* 7:127 (1993)).

In yet another embodiment, the suitability of inhibitor candidates can be determined using an empirical scoring function, which can rank the binding affinities for a set of inhibitors. For an example of such a method see Muegge *et al.* and references therein (Muegge *et al.*, *J Med. Chem.* **42**:791-804 (1999)).

Other modeling techniques can be used in accordance with this invention, for example, those described by Cohen *et al.* (*J. Med. Chem.* **33**: 883-894 (1994)); Navia *et al.* (*Current Opinions in Structural Biology* **2**: 202-210 (1992)); Baldwin *et al.* (*J. Med. Chem.* **32**: 2510-2513 (1989)); Appelt *et al.* (*J. Med. Chem.* **34**: 1925-1934 (1991)); and Ealick *et al.* (*Proc. Nat. Acad. Sci. USA* **88**: 11540-11544 (1991)).

A compound which is identified by one of the foregoing methods as a potential inhibitor of Tie-2 can then be obtained, for example, by synthesis or from a compound library, and assessed for the ability to inhibit Tie-2 *in vitro*. Such an *in vitro* assay can be performed as is known in the art, for example, by contacting Tie-2 in solution with the test compound in the presence of a substrate for Tie-2. The rate of substrate transformation can be determined in the presence of the test compound and compared with the rate in the absence of the test compound. Suitable assays for Tie-2 biological activity are described in Example 4.

An inhibitor identified or designed by a method of the present invention can be a competitive inhibitor, an uncompetitive inhibitor or a noncompetitive inhibitor. A "competitive" inhibitor is one that inhibits Tie-2 activity by binding fully or partially within the same region of Tie-2, as ATP, thereby directly competing with ATP for the active site of Tie-2. An "uncompetitive" inhibitor inhibits Tie-2 by binding to a different region of the enzyme than ATP. Such inhibitors bind to Tie-2 already bound with ATP and not to the free enzyme. A "non-competitive" inhibitor is one that can bind to either the free or ATP bound form of Tie-2. In some instances, an inhibitor may inhibit the enzymes catalytic activity by impeding the binding of multiple substrates (e.g., ATP and tyrosyl substrates). this may be accomplished by fully or partially occluding multiple substrate binding sites, or by occupying a site which allosterically or conformationally reduces affinities for substrates or blocks product release.

In another embodiment, the present invention provides Tie-2 inhibitors, and methods of use thereof, which are capable of binding to the catalytic domain of Tie-2, for example, compounds which are identified as inhibitors of at least one biological activity of Tie-2 or which are designed by the methods described above to inhibit at least one biological activity of Tie-2. For example, the invention includes compounds which interact with one or more, preferably two or more, and more preferably, three or more of Tie-2 subsites 1 to 9.

In one embodiment, the Tie-2 inhibitor of the invention comprises a moiety or moieties positioned to interact with subsite 1, subsite 2 and, optionally, with at least one other subsite, when present in the Tie-2 catalytic domain. For example, a

functional group which can interact with subsite 1 can be a hydrogen bond donor, a hydrogen bond acceptor, or a hydrophobic moiety. A functional group which can interact with subsite 2 can be a hydrophobic group, hydrogen bond donor, or a hydrogen bond acceptor.

In another embodiment, the Tie-2 inhibitor of the invention comprises functional groups positioned to interact with subsites 1, 2 and 3, and, optionally, one or more additional subsites.

The Tie-2 inhibitors of the invention also include compounds having functional groups positioned to interact with subsite 1, subsite 2, subsite 8 and, optionally, one or more additional subsites. In another embodiment, the inhibitor has functional groups positioned to interact with subsite 1, subsite 2, subsite 3, subsite 8, and, optionally, one or more additional subsites.

In other embodiments, the Tie-2 inhibitors of the invention include compounds which have functional groups positioned to interact with the following groups of subsites, each of which can, optionally, include one or more additional subsites: subsites 1, 4, and 5; subsites 1, 2, 7 and 8; subsites 1, 2, 3, 7 and 8; subsites 1, 2, 3, 7 and 8; subsites 1, 2, 4, 6 and 8; subsites 1, 2, 3, 4, 6 and 8; subsites 1, 2, 3, 4, 6 and 8.

A moiety of the inhibitor compound is "positioned to interact" with a given subsite, if, when placed within the Tie-2 catalytic domain, as defined by the atomic coordinates presented in Figs. 3-6, the moiety is proximal to, and oriented properly relative to, the appropriate amino acid side chains within the subsite.

As indicated in the description of the subsites above, several of subsites 1-9 can potentially interact with two or more types of moieties. For each of the subsites listed below the preferred type of interacting moiety possessed by the potential inhibitor is indicated.

Subsite 1: hydrogen bond donor (E903) and hydrogen bond acceptor (A905).

Subsite 2: hydrophobic, preferably aromatic, moiety (I830, V838, I886, I902 and L971).

Subsite 3: hydrophobic, preferably alkyl, moiety (I830 and L971) and a positively charged moiety (D912).

Subsite 4: hydrogen acceptor moiety (D982 and F938).

Subsite 8: hydrophobic, preferably aromatic, moiety (L876, I886, L888 and F983)

A preferred Tie-2 inhibitor of the invention inhibits Tie-2 enzymatic activity with a Ki of at least about 1 mM, preferably at least about 100 μM and more preferably at least about 10 μM. In another embodiment, a Tie-2 inhibitor binds selectively to a Tie-2 receptor over other tyrosine kinase receptors, such as insulin receptor or Csk, KDR, lck, or zap. In a preferred embodiment, the inhibitor has a K_i 0.1 fold or less for a Tie-2 receptor than for an insulin receptor or Csk. In a more preferred embodiment, the inhibitor has K_i 0.01 fold or less for a Tie-2 receptor than for an insulin receptor or Csk. In a most preferred embodiment, the inhibitor has an K_i 0.001 fold less or less for a Tie-2 receptor than for an insulin receptor or Csk.

In a preferred embodiment, the Tie-2 inhibitor of the invention comprises two or more of the following when present at, or bound to, the Tie-2 catalytic domain: (a) a hydrogen bond donor positioned to interact with Glu 903 of human Tie-2; (b) a hydrogen bond acceptor positioned to interact with Ala 905 of human Tie-2; (c) a hydrogen bond donor positioned to interact with Ala 905 of human Tie-2; (d) a hydrophobic moiety positioned to interact with one or more of Ile 830, Val 838, Ala 853, Ile 886, Ile 902, Tyr 904, Ala 905 and Leu 971 of human Tie-2; (e) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 912 of human Tie-2; (f) a hydrogen bond donor or hydrogen bond acceptor postioned to interact with Asn 909 of human Tie-2; (g) a hydrophobic moiety positoned to interact with one or more of Val 838, Lys 855, Ile 886, Ile 902, Leu 971 and Ala 981 of human Tie-2; (h) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 855 of human Tie-2; (i) a hydrogen bond acceptor positioned to interact with Asp 982 of human Tie-2; (j) a hydrogen bond acceptor

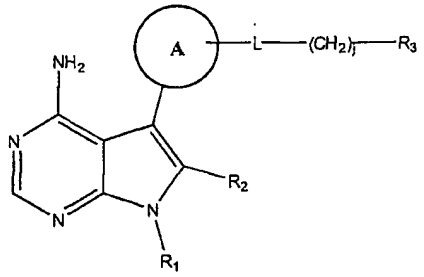
positioned to interact with Phe 983 of human Tie-2; (k) a hydrophobic moiety positioned to interact with one or more of Leu 873, Leu 876, Ile 885, Ile 886, Leu 888, Leu 900, Ile 902, Ala 981 and Phe 983 of human Tie-2; (l) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 982 of human Tie-2; (m) a hydrogen bond donor positioned to interact with Ile 886 of human Tie-2; (n) a hydrogen bond donor positioned to interact with Leu 768 of human Tie-2; (o) a hydrogen bond acceptor positioned to interact with Gly 831 of human Tie-2; (p) a hydrogen bond donor or positively charged functional group positioned to interact with Glu 832 of human Tie-2; (q) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 840 of human Tie-2; (r) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 916 of human Tie-2; (s) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Arg 968 of human Tie-2; (t) a hydrogen bond donor positioned to interact with Arg 968 of human Tie-2.

In preferred embodiments, the Tie-2 inhibitors of the invention comprise (b) and (d); (d) and at least one of (a), (b) and (c); (d) and at least two of (a), (b) and (c); (d) and at least two of (a), (b) and (c), and at least one of (e) and (f); (d) and (g), and at least two of (a), (b) and (c); (d), (g), at least two of (a), (b) and (c) and at least one of (e) and (f); (d), (g), (k), and at least two of (a), (b) and (c); (d), (g), (k), at least one of (e) and (f), at least two of (a), (b), and (c); (d), at least one of (i) and (j), and at least two of (a), (b) and (c); (d) and at least two of (a), (b) and (c), at least one of (e) and (f), and at least one of (i) and (j); (d), (g), (k), at least one of (i) and (j), and at least two of (a), (b) and (c); and (d), (g), (k), at least one of (e) and (f), and at least two of (a), (b) and (c).

Preferred Tie-2 inhibitors of the invention comprise a molecular scaffold or framework, to which the moieties and/or functional groups which interact with the Tie-2 subsites are attached, either directly or via an intervening moiety. The scaffold can be, for example, a peptide or peptide mimetic backbone, a cyclic or polycyclic moiety, such as a monocyclic, bicyclic or tricyclic moiety, and can include one or more hydrocarbonyl or heterocyclic rings. The molecular scaffold presents the

attached interacting moieties in the proper configuration or orientation for interaction with the appropriate residues of Tie-2.

Pyrrolopyrimidines, such as inhibitor, I, II, III or IV, are preferred Tie-2 inhibitors. Methods for synthesizing pyrrolopyrimidines are described in PCT application number WO99/21560, the teachings of which are incorporated herein by reference in their entirety. In one embodiment, the inhibitors of the invention do not include the pyrrolopyrimidines represented by structural formula V:



V.

and pharmaceutically acceptable salts thereof, wherein:

Ring A is a six membered aromatic ring or a five or six membered heteroaromatic ring which is optionally substituted with one or more substituents selected from the group consisting of a substituted or unsubstituted aliphatic group, a halogen, a substituted or unsubstituted aromatic group, substituted or unsubstituted heteroaromatic group, substituted or unsubstituted cycloalkyl, substituted or unsubstituted heterocycloalkyl, substituted or unsubstituted aralkyl, substituted or unsubstituted heteroaralkyl, cyano, nitro, $-NR_4R_5$, $-C(O)_2H$, -OH, a substituted or unsubstituted alkoxycarbonyl, $-C(O)_2$-haloalkyl, a substituted or unsubstituted alkylthio ether, a substituted or unsubstituted alkylsulfoxide, a substituted or unsubstituted alkylsulfone, a substituted or unsubstituted arylthio ether, a substituted or unsubstituted arylsulfoxide, a substituted or unsubstituted arylsulfone, a substituted or unsubstituted alkyl carbonyl, -C(O)-haloalkyl, a substituted or unsubstituted aliphatic ether, a substituted or unsubstituted aromatic ether, carboxamido, tetrazolyl, trifluoromethylsulphonamido,

trifluoromethylcarbonylamino, a substituted or unsubstituted alkynyl, a substituted or unsubstituted alkyl amido, a substituted or unsubstituted aryl amido, -$NR_{95}C(O)R_{95}$, a substituted or unsubstituted styryl and a substituted or unsubstituted aralkyl amido, wherein R_{95} is an aliphatic group or an aromatic group;

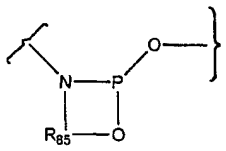
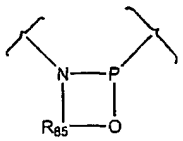
L is -O-; -S-; -S(O)-; -$S(O)_2$-; -N(R)-; -N(C(O)OR)-; -N(C(O)R)-; -$N(SO_2R)$; -CH_2O-; -CH_2S-; -$CH_2N(R)$-; -CH(NR)-;-$CH_2N(C(O)R)$)-; -$CH_2N(C(O)OR)$-; -$CH_2N(SO_2R)$-; -CH(NHR)-; -CH(NHC(O)R)-; -$CH(NHSO_2R)$-; -CH(NHC(O)OR)-;-CH(OC(O)R)-;-CH(OC(O)NHR)-; -CH=CH-; -C(=NOR)-;

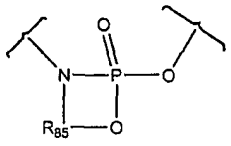
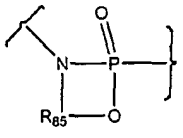
-C(O)-; -CH(OR)-;-C(O)N(R)-; -N(R)C(O)-; -N(R)S(O)-;-$N(R)S(O)_2$-; -OC(O)N(R)-;-N(R)C(O)N(R)-; -NRC(O)O-;-S(O)N(R)-;-$S(O)_2N(R)$-; N(C(O)R)S(O)-; $N(C(O)R)S(O)_2$-; -N(R)S(O)N(R)-; -$N(R)S(O)_2N(R)$-; -C(O)N(R)C(O)-; -S(O)N(R)C(O)-; -$S(O)_2N(R)C(O)$-; -OS(O)N(R)-; -$OS(O)_2N(R)$-; -N(R)S(O)O-; -$N(R)S(O)_2O$-; -N(R)S(O)C(O)-; -$N(R)S(O)_2C(O)$-; -SON(C(O)R)-; -$SO_2N(C(O)R)$-; -N(R)SON(R)-; -$N(R)SO_2N(R)$-; -C(O)O-;

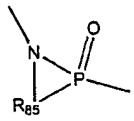
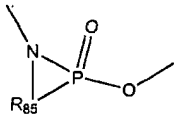
-N(R)P(OR')O-; -N(R)P(OR')-; -N(R)P(O)(OR')O-; -N(R)P(O)(OR')-; -N(C(O)R)P(OR')O-; -N(C(O)R)P(OR')-; -N(C(O)R)P(O)(OR')O- or -N(C(O)R)P(OR')-, wherein R and R' are each, independently, -H, an acyl group, a substituted or unsubstituted aliphatic group, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic group, or a substituted or unsubstituted cycloalkyl group; or

L is –R_bN(R)$S(O)_2$-, -R_bN(R)P(O)-, or -R_bN(R)P(O)O-, wherein R_b is an alkylene group which when taken together with the sulphonamide, phosphinamide, or phosphonamide group to which it is bound forms a five or six membered ring fused to ring A; or

L is represented by one of the following structural formulas:


or


wherein R_{85} taken together with the phosphinamide, or phophonamide is a 5-, 6-, or 7-membered, aromatic, heteroaromatic or heterocycloalkyl ring system;

R_1 is a substituted aliphatic group, a substituted cycloalkyl, a substituted bicycloalkyl, a substituted cycloalkenyl, an optionally substituted aromatic group, an optionally substituted heteroaromatic group, an optionally substituted heteroaralkyl, an optionally substituted heterocycloalkyl, an optionally substituted heterobicycloalkyl, an optionally substituted alkylamindo, and optionally substituted arylamido, an optionally substituted -$S(O)_2$-alkyl or optionally substituted -$S(O)_2$-cycloalkyl, a -C(O)-alkyl or an optionally substituted –C(O)-alkyl, provided that when R_1 is an aliphatic group or cycloalkyl group, R_1 is not exclusively substituted with one or more substitutent selected from the group consisting of hydroxyl and lower alkyl ethers, provided that the heterocycloalkyl is not 2-phenyl-1,3-dioxan-5-yl and

provided that an aliphatic group is not substituted exclusively with one or more aliphatic groups, wherein one or more substituent is selected from the group consisting of a substituted or unsubstituted aliphatic group, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic, a substituted or unsubstituted aralkyl, a substituted or unsubstituted heteroaralkyl, a substituted or unsubstituted cycloalkyl, a substituted or unsubstituted heterocycloalkyl, a substituted or unsubstituted aromatic ether, a substituted or unsubstituted aliphatic ether, a substituted or unsubstituted alkoxycarbonyl, a substituted or unsubstituted alkylcarbonyl, a substituted or unsubstituted arylcarbonyl, a substituted or unsubstituted heteroarylcarbonyl, substituted or unsubstituted aryloxycarbonyl, -OH, a substituted or unsubstituted aminocarbonyl, an oxime, a substituted or unsubstituted azabicycloalkyl, heterocycloalkyl, oxo, aldehyde, a substituted or unsubstituted alkyl sulfonamido group, a substituted or unsubstituted aryl sulfonamido group, a substituted or unsubstituted bicycloalkyl, a substituted or unsubstituted heterobicycloalkyl, cyano, $-NH_2$, an alkylamino, ureido, thioureido and –B-E;

B is a substituted or unsubstituted cycloalkyl, a substituted or unsubstituted heterocycloalkyl, a substituted or unsubstituted aromatic, a substituted or unsubstituted heteroaromatic, an alkylene, an aminoalkyl, an alkylenecarbnonyl, or an aminoalkylcarbonyl;

E is a substituted or unsubstituted azacycloalkyl, a substituted or unsubstituted azacycloalkylcarbonyl, a substituted or unsubstituted azacycloalkylsulfonyl, a substituted or unsubstituted azacycloalkylalkyl, a substituted or unsubstituted heteroaryl, a substituted or unsubstituted heteroarylcarbonyl, a substituted or unsubstituted heteroarylsulfonyl, a substituted or unsubstituted heteroaralkyl, a substituted or unsubstituted alkyl sulfonamido, a substituted or unsubstituted aryl sulfonamido, a substituted or unsubstituted bicycloalkyl, a substituted or unsubstituted ureido, a substituted or unsubstituted thioureido or a substituted or unsubstituted aryl;

R_2 is –H, a substituted or unsubstituted aliphatic group, a substituted or unsubstituted cycloalkyl, a halogen, -OH, cyano, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic group, a substituted or unsubstituted heterocycloalkyl, a substituted or unsubstituted aralkyl, a substituted or unsubstituted heteroaralkyl, $-NR_4R_5$, or $-C(O)NR_4R_5$;

R_3 is a substituted or unsubstituted aliphatic group, a substituted or unsubstituted alkenyl group, a substituted or unsubstituted cycloalkyl, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic group, or a substituted or unsubstituted heterocycloalkyl;

provided that L is $-SN(R)-$, $-S(O)N(R)-$, $-S(O)_2N(R)-$, $-N(R)S-$, $-N(R)S(O)-$, $-N(R)S(O)_2-$, $-N(R)SN(R')-$, $-N(R)S(O)N(R')-$, or $-N(R)S(O)_2N(R')-$ when R_3 is a substituted or unsubstituted aliphatic group, a substituted or unsubstituted alkenyl group;

provided that *j* is 0 when L is –O-, $-CH_2NR-$, -C(O)NR- or –NRC(O)- and R_3 is azacycloalkyl or azaheteroaryl; and

provided that j is 0 when L is –O- and R_3 is phenyl;

R_4, R_5 and the nitrogen atom together form a 3, 4, 5, 6 or 7-membered, substituted or unsubstituted heterocycloalkyl, substituted or unsubstituted heterobicycloalkyl or a substituted or unsubstituted heteroaromatic; or

R_4 and R_5 are each, independently, -H, azabicycloalkyl, heterocycloalkyl, a substituted or unsubstituted alkyl group or Y-Z;

Y is selected from the group consisting of $-C(O)-$, $-(CH_2)_p-$, $-S(O)_2-$, $-C(O)O-$, $-SO_2NH-$, -CONH-, $(CH_2)_pO-$, $-(CH_2)_pNH-$, $-(CH_2)_pS-$, $-(CH_2)_pS(O)-$, and $-(CH_2)_pS(O)_2-$;

p is an integer from 0 to 6;

Z is –H, a substituted or unsubstituted alkyl, substituted or unsubstituted amino, substituted or unsubstituted aryl, substituted or unsubstituted heteroaryl or substituted or unsubstituted heterocycloalkyl group; and

j an integer from 0 to 6.

As used herein, aromatic groups include carbocyclic ring systems (e.g. phenyl

and cinnamyl) and fused polycyclic aromatic ring systems (e.g. naphthyl and 1,2,3,4-tetrahydronaphthyl). Arromatic groups are also referred to as aryl groups herein.

Heteroaromatic groups, as used herein, include heteroaryl ring systems (e.g., thienyl, pyridyl, pyrazole, isoxazolyl, thiadiazolyl, oxadiazolyl, indazolyl, furans, pyrroles, imidazoles, pyrazoles, triazoles, pyrimidines, pyrazines, thiazoles, isoxazoles, isothiazoles, tetrazoles, or oxadiazoles) and heteroaryl ring systems in which a carbocyclic aromatic ring, carbocyclic non-aromatic ring or heteroaryl ring is fused to one or more other heteroaryl rings (e.g., benzo(b)thienyl, benzimidazole, indole, tetrahydroindole, azaindole, indazole, quinoline, imidazopyridine, purine, pyrrolo[2,3-d]pyrimidine, pyrazolo[3,4-d]pyrimidine) and their N-oxides.

An aralkyl group, as used herein, is an aromatic substituent that is linked to a compound by an aliphatic group having from one to about six carbon atoms.

An heteroaralkyl group, as used herein, is a heteroaromatic substituent that is linked to a compound by an aliphatic group having from one to about six carbon atoms.

A heterocycloalkyl group, as used herein, is a non-aromatic ring system that has 3 to 8 atoms and includes at least one heteroatom, such as nitrogen, oxygen, or sulfur.

An acyl group, as used herein, is an $-C(O)NR_xR_z$, $-C(O)OR_x$, $-C(O)R_x$, in which R_x and R_z are each, independently, -H, a substituted or unsubstituted aliphatic group or a substituted or unsubstituted aromatic group.

As used herein, aliphatic groups include straight chained, branched or cyclic C_1-C_8 hydrocarbons which are completely saturated or which contain one or more units of unsaturation. A "lower alkyl group" is a saturated aliphatic group having form 1-6 carbon atoms.

Inhibitor I bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 3 for atomic coordinates) crystallized in the space group C2221. The x-ray crystallographic structure reveiled the following interactions:

The pyrrolopyrimidine ring of the inhibitor I forms hydrogen bonds to residues in the hinge region and interacts with purine core region. The core of the inhibitor presents a hydrogen bond donor in the form of the amino proton of the 4-NH_2

substituent to the carbonyl oxygen of E903. Atom N3 of the pyrimidine ring accepts a hydrogen bond from the backbone N-H of A905. The ring system of the core presents a planar face to residues of both the C-terminal and N-terminal lobes. The residues in these areas present a hydrophobic surface which "sandwiches" the planar core of the inhibitor. Residues involved in this hydrophobic sandwich region include I830, V838, I86, I902 and L971. Atoms N1 and N7 of the core face the solvent exposed mouth of the binding pocket. Atom C6 faces the long axis of the nucleotide binding loop of the N-terminal lobe of the protein.

The N7 cyclopentane ring is directed towards solvent but is still within the protein cavity. This region was described above as the extended sugar pocket after the binding mode of the ribose ring of ATP observed in other kinase structures. This region is characterized by hydrophobic interactions with primarily I830 and L971. Methylene groups of E832 may also contribute in this fashion.

The phenyl ring attached to C5 of the pyrrolopyrimidine ring is in a predominantly hydrophobic area, generated by residues from the purine core region, the distal hydrophobic pocket and methylene groups from the catalytic lysine, K855. The hydrophobic contacts are with residues V838, I886, I902, L971 and A981. Lysine 855 is highly mobile, so it is also possible that the Cl atom meta to the pyrrolopyrimidine ring is receiving a hydrogen bond.

The sulfonamide linker makes a clear hydrogen bond with an amide proton of D982 and may also make a hydrogen bond to the amide proton of F983.

The terminal phenyl ring (labelled ring C) is located in the distal hydrophobic pocket. Primary contacts are with L876, I886, L888 and F983.

Inhibitor II bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 4 for atomic coordinates) crystallized in the space group P42212. The x-ray crystallographic structure reveiled the following additional interactions:

The pyrrolopyrimidine core, B-ring, linker and C-ring bind the same way as inhibitor I. The N-7 cyclohexyl N-methy piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912.

Inhibitor III bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 4 for atomic coordinates) crystallized in the space group P42212.

The x-ray crystallographic structure reveiled the following additional interactions:

The pyrrolopyrimidine core binds the same way as inhibitor I. The N-7 cyclohexyl N-methy piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912 as in Tie-2/inhibitor II. The B-ring binds in a similar fashion to inhibitor I, however, the hydrogen bond between a halogen, fluorine in this case, and K855 is more clear. The linker makes two clear hydrogen bonds to backbone amide protons of D983 and F983. The C-ring occupies the distal hydrophobic pocket with main interactions coming from L876, I886, L888, L900, I902 and F983.

Inhibitor IV bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 4 for atomic coordinates) crystallized in the space group P42212. The x-ray crystallographic structure reveiled the following additional interactions:

The pyrrolopyrimidine core binds the same way as inhibitor I. The N-7 cyclohexyl N-methy piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912 as in Tie-2/inhibitor II. The B-ring binds in a similar fashion to inhibitor I, however there is no chlorine atom to act as a potential hydrogen bond partner. The linker in this case is an oxygen atom which accepts a hydrogen bond from the catalytic lysine, K855. The C-ring occupies the distal hydrophobic pocket with main interactions coming from L876, I886, I902 and F983.

In one embodiment, the present invention relates to a method of treating a Tie-2-dependent condition in a patient. The method comprises the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor as described above. The patient can be any animal, and is, preferably, a mammal and, more preferably, a human.

A "Tie-2-dependent condition" is a disease or medical condition in which the catalytic activity of Tie-2 plays a role, for example, in the development of the disease or condition. For example, in one embodiment, the condition is characterized by excessive vascular proliferation. Tie-2 inhibitors are useful in treating angiogenesis dependent disorders, and disorders involving aberrant endothilial-pereindothelial interactions (e.g., restenosis).

Tie-2 dependent conditions include hyperproliferative disorders, cancer, a cardiovascular condition, an ocular condition, von Hippel Lindau disease, pemphigoid, psoriasis, Paget's disease, polycystic kidney disease, fibrosis, sarcoidosis, cirrhosis, thyroiditis, Osler-Weber-Rendu disease, chronic inflammation, synovitis, inflammatory bowel disease, Crohn's disease, rheumatoid arthritis, osteoarthritis, psoriatic arthritis, an ulcer and sepsis. In addition a Tie-2 inhibitor can be used to decrease fertility in a patient.

Preferred methods of treatment are where the cancer is a solid tumor, a sarcoma, fibrosarcoma, osteoma, melanoma, retinoblastoma, a rhabdomyosarcoma, glioblastoma, neuroblastoma, teratocarcinoma, an hematopoietic malignancy, malignant ascites, Kaposi's sarcoma, Hodgkin's disease, lymphoma, myeloma or leukemia.

Another preferred method of treatment is where the cardiovascular condition, atherosclerosis, restenosis, ischemia/reperfusion injury, chronic occlusive pulmonary disease, vascular occlusion, carotid obstructive disease, Crow-Fukase (POEMS) syndrome, anemia, ischemia, infarct, vascular leakage disorders.

Yet another preferred method of treatment is where the ocular condition is ocular or macular edema, ocular neovascular disease, scleritis, radial keratotomy, uveitis, vitritis, myopia, optic pits, chronic retinal detachment, post-laser treatment complications, conjunctivitis, Stargardt's disease, Eales disease, retinopathy, macular degeneration or microangiopathy.

A Tie-2 inhibitor can also be used in a method of promoting angiogenesis or vasculogenesis. In addition, a Tie-2 inhibitor can be administered with a pro-angiogenic growth factor.

A therapeutically effective amount, as this term is used herein, is an amount which results in partial or complete inhibition of disease progression or symptoms. Such an amount will depend, for example, on the size and gender of the patient, the condition to be treated, the severity of the symptoms and the result sought, and can be determined by one skilled in the art.

The compound of the invention can, optionally, be administered in combination with one or more additional drugs or therapies which, for example, are

known for treating and/or alleviating symptoms of the condition mediated by Tie-2. The additional drug can be administered simultaneously with the compound of the invention, or sequentially. For example, the Tie-2 inhibitor can be administered in combination with another anticancer agent, as is known in the art. Additional therapies which may be coadministered would include, for example, radiation therapy, ultraviolet irradiation, hyperthermia, laser irradiation, targeted radionuclides and neutron bombardment.

The invention further provides pharmaceutical compositions comprising one or more of the Tie-2 inhibitors described above. Such compositions comprise a therapeutically (or prophylactically) effective amount of one or more Tie-2 binding inhibitors, as described above, and a pharmaceutically acceptable carrier or excipient. Suitable pharmaceutically acceptable carriers include, but are not limited to, saline, buffered saline, dextrose, water, glycerol, ethanol, and combinations thereof. The carrier and composition can be sterile. The formulation should suit the mode of administration.

Suitable pharmaceutically acceptable carriers include but are not limited to water, salt solutions (e.g., NaCl), alcohols, gum arabic, vegetable oils, benzyl alcohols, polyethylene glycols, gelatin, carbohydrates such as lactose, amylose or starch, cyclodextrin, magnesium stearate, talc, silicic acid, viscous paraffin, perfume oil, fatty acid esters, hydroxymethylcellulose, polyvinyl pyrolidone, etc. The pharmaceutical preparations can be sterilized and if desired, mixed with auxiliary agents, e.g., lubricants, preservatives, stabilizers, wetting agents, emulsifiers, salts for influencing osmotic pressure, buffers, coloring, flavoring and/or aromatic substances and the like which do not deleteriously react with the active compounds.

The composition, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents. The composition can be a liquid solution, suspension, emulsion, tablet, pill, capsule, sustained release formulation, or powder. The composition can be formulated as a suppository, with traditional binders and carriers such as triglycerides. Oral formulation can include standard carriers such as pharmaceutical grades of mannitol, lactose, starch, magnesium stearate, polyvinyl pyrrolidinone, sodium saccharine, cellulose, magnesium carbonate, etc.

The composition can be formulated in accordance with the routine procedures as a pharmaceutical composition adapted for intravenous administration to human beings. Typically, compositions for intravenous administration are solutions in sterile isotonic aqueous buffer. Where necessary, the composition may also include a solubilizing agent and a local anesthetic to ease pain at the site of the injection. Generally, the ingredients are supplied either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachet indicating the quantity of active agent. Where the composition is to be administered by infusion, it can be dispensed with an infusion bottle containing sterile pharmaceutical grade water, saline or dextrose/water. Where the composition is administered by injection, an ampoule of sterile water for injection or saline can be provided so that the ingredients may be mixed prior to administration.

The pharmaceutical compositions of the invention can also include an agent which controls release of the Tie-2 inhibitor compound, thereby providing a timed or sustained release composition.

The Tie-2 inhibitor can be administered subcutaneously, intravenously, parenterally, intraperitoneally, intradermally, intramuscularly, intraocularly, topically, enteral (e.g., orally), rectally, nasally, buccally, sublingually, vaginally, by inhalation spray, by drug pump or via an implanted reservoir in dosage formulations containing conventional non-toxic, physiologically acceptable carriers or vehicles. The preferred method of administration is by oral delivery. The form in which it is administered (e.g., syrup, elixir, capsule, tablet, solution, foams, emulsion, gel, sol) will depend in part on the route by which it is administered. For example, for mucosal (e.g., oral mucosa, rectal, ocular mucosa, intestinal mucosa, bronchial mucosa) administration, nose drops, aerosols, inhalants, nebulizers, eye drops or suppositories can be used. The compounds and agents of this invention can be administered together with other biologically active agents, such as analgesics, anti-inflammatory agents, anesthetics and other agents which can control one or more symptoms or causes of a Tie-2 dependent condition.

In a specific embodiment, it may be desirable to administer the agents of the invention locally to a localized area in need of treatment; this may be achieved by, for example, and not by way of limitation, local infusion during surgery, topical application, transdermal patches, by injection, by means of a catheter, by means of a suppository, or by means of an implant, said implant being of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes or fibers. For example, the agent can be injected into the joints.

EXAMPLES

Example 1 Protein Purification

$(His)_6$Tie-2 802-1124, D964N, which contains a TEV protease cleavage peptide, was expressed recombinantly by baculovirus infection of SF-9 cells. Cells were lysed in a buffer containing 20 mM Tris pH 8.0, 137 mM NaCl , 10 % glycerol, 1 % Triton X-100, 1 mM ADP, 5 mM $MgCl_2$ and complete protease inhibitor, EDTA-free cocktail from Boehringer Mannhein.. The ligand ADP/Mg^{++} was maintained at this concentration in buffers of all subsequent purification steps. The cell lysate was centrifuged and the supernatant was applied to a Ni^{++} chelating sepharose column which had been equilibrated in 50 mM HEPES, pH 7.5, 0.3 M NaCl. Tie-2 was eluted by competition with 100 mM imidazole. The eluted $(His)_6$ Tie-2 was digested with Tev protease and dialyzed against 50 mM HEPES, pH 7.5, 0.25 M NaCl, 5 mM DTT. The dialyzed sample was centrifuged to remove any precipitated protein, and Tie-2 was bound to a MonoQ anion exchange column and eluted with a linear 20 column volume gradient of 0.025-0.2 M NaCl. Typically, differences in the monodispersity of early eluting verses late eluting fractions could be detected using Dynamic Light Scattering (DLS). Sample purity was assessed with SDS-PAGE, native PAGE, and LC/MS total mass analysis. Fractions with similar DLS characteristics were pooled and concentrated to greater than 2 mg/ml using ultrafiltration at –80 ^{0}C. The ultracentrifuged samples were used in crystallographic

experiments described below. Table I lists a range of conditions suitable for crystallization.

Example 2:

I. Diphosphorylated Tie-2 802-1124

A. Crystallization Conditions:

Tie-2 802-1124 ($2PO_4$) protein was crystallized in a sitting or hanging drop geometry using a vapor diffusion method. The protein concentration was 5 mg/ml, and the well solution was 10% PEG 6,000; 0.1 M HEPES, pH 7.5; 5% MPD (2-methyl-2,4-pentanediol). Drops were set up using equal volumes of protein and well solution containing 500 μM inhibitor. Crystals routinely grew to 0.4 mm x 0.1 mm x 0.01 mm in about a week. Crystals were of the space group P2(1)2(1)2(1) with unit cell dimensions a = 54.320 Å, b = 75.872 Å, c = 78.143 Å , and $\alpha = \beta = \gamma = 90.0^{o}$. Table I list a range of conditions which are suitable for crystallization.

B. Data Collection

Data on ligand bound crystals were collected on a Rigaku RU300 rotating anode generator running at 50kV 150 mA equipped with an R-Axis II phosphoimage plate detector. X-rays were monochromatized by long mirrors and filtered with a 0.0067μm Nickel filter. Data were processed and reduced with DENZO and SCALEPACK (Minor, W. 1993). Data were collected to 3.5 Å resolution.

C. Data Processing

Programs in the CCP4 suite (Collaborative Computational Project, Number 4 1994) (tomtz, trunc, cad and ecalc) were used to format and process the data for molecular replacement. The molecular replacement program AMORE (Navaza, J. 1994) was used successfully to find phases for the data set using an initial model. The initial model was composed of the carboxy-terminal portion (residues 566-575 and 592-672) of the FGFR kinase domain trimmed back to poly-Alanine (PDB accession number 1FGK). A second round of AMORE with a more complete model (residues

464-485, 491-500, 505-575 and 592-762) was also performed to confirm the phasing solution.

D. Optimization of Model

Several round of least-squared minimization using CNS (Brunger, A.T. et al., 1998) alternating with manual rebuilding, using the graphics program O, version 6.2.1 (Jones, A., 1997; Kleywegt G. J., 1995) were performed iteratively to improve the model while comparing it to electron density maps generated after each round with coefficients 2fo-fc contoured at a level of 1.0 sigma.

II. Tie-2 (D964N) 802-1124 (SEQ ID NO 2)

A. Crystallization Conditions

Purified Tie-2 (D964N) 802-1124 protein was crystallized in a sitting drop geometry using the vapor diffusion method. The protein concentration was 2.5 mg/ml, and the well solution was 1.0 to 1.5 M ammonium sulfate, 0.1M MES, pH 6.5, 5% dioxane (1,4-dioxane). Drops were set up using equal volumes of protein and well solution containing 100-300 μM inhibitor. Crystals routinely grew to 0.3 mm x 0.05 mm x 0.01 mm in about 2-3 days. Crystals of Tie-2/inhibitor I were of the space group C222(1) with unit cell dimensions a = 75.195 Å, b = 116.287 Å, c = 95.060 Å and $\alpha = \beta = \gamma$ - 90.0°. Crystals of the Tie-2/inhibitor II, III or IV complex were of the space group P42212 with unit cell dimensions a = b = 86.0 Å, c = 112.0 Å and $\alpha = \beta = \gamma$ - 90.0°.

B. Data Collection

Data on a ligand-bound crystal (Tie-2 (D964N) 802-1124) complexed with inhibitors I, II, III, or IV were collected at the beamline X25 at Brookhaven National Laboratory (Upton, NY) equipped with the Brandeis B4, CCD detector. Data were processed and reduced with DENZO and SCALEPACK (Minor, W. 1993). Data for the Tie-2/inhibitor I complex were collected complete to 2.75 Å resolution, with higher resolution reflections visible to 2.0 Å resolution.

C. Data Processing

Programs in the CCP4 suite (Collaborative Computational Project, Number 4 1994) (tomtz, trunc, cad and ecalc) were used to format and process the data for molecular replacement. The molecular replacement program AMORE (Navaza, J. 1994) was used successfully to find phases for the data set using an initial model. The initial model was composed of the a conservative portion of the FGFR kinase domain (Tie2 residue numbering 818-830, 841-842, 850-857, 866-890, 900-916, 935-981, 1001-1093). The model, mostly poly-Alanine, was trimmed of loop regions which diverged upon superposition of five tyrosine kinase structures (IRK, HCK, SRC, FGFR, and LCK). In addition this model included only those side-chain residues in positions where an identical side-chain was found in the FGFR model.

D. Optimization of Model

Several round of least-squared minimization using CNS (Brunger, A. T. et al., 1998) alternating with manual rebuilding, using the graphics program O, version 6.2 (Jones, A., 1997; Kleywegt G. J., 1995) were performed to iteratively improve the model while comparing it to two electron density maps: one generated with coefficients 2fo-fc contoured at a level of 1.0 sigma and the other generated with coefficients fo-fc contoured at a level of 1.5 sigma.

E. Inhibitor Docking

Inhibitor I was found to be bound to the active site. It was initially docked by hand in O by visually inspecting the electron density maps and adjusting the torsion angles of the inhibitor. Parameter and topology files were generated for CNS using the X-util program xplo2d (Kleywegt G. J. and Jones, T.A. 1997) and modified slightly to properly model chlorine in the inhibitor.

III. Tie-2 (D964N) 802-1124 (SEQ ID NO 2)

A. Crystallization Conditions

The protein (construct Tie-2D964N) was provided in a buffer containing 25mM HEPES, pH 7.5, 50 mM NaCl, 5 mM MgCl2, 1 mM ADP and 5 mM DTT. The protein concentration was about 2.3 mg/ml as determined with a Coomassie Plus assay, BSA as standard.

The inhibitor III was dissolved in DMSO to give a 50 mM stock solution. Stock solution was added to the protein solution for a final inhibitor concentration of 2mM. Crystallization conditions were screened with Hampton Screen *Crystal screen, Crystal screen2, Membfac, Natrix* and *PEG/ion screen* at room temperature and 4°C. Crystals grew with precipitation buffer: 20% PEG 3350, 0,2M tri-Lithium Citrat pH 8,1 (Hampton Screen *PEG/ion screen*, Nr. 45) sitting or hanging drop: 750µl buffer in reservoir in the drop typically 1µl - 2µl protein and 1µl - 2µl reservoir solution were mixed.

Addition of the following additives (10% by volume to the drop) also yielded crystals:

Add. Screen I Nr.:01	0.1M Ba-Chloride
Add. Screen I Nr.:03	0.1M Ca-Chloride
Add. Screen I Nr.:06	0.1M Mg-Chloride
Add. Screen I Nr.:16	0.1M Trimehylamine
Add. Screen I Nr.:22	30% Ethanol
Add. Screen II Nr.:08	30% Xylitol
Add. Screen II Nr.:13	30% 1,5Diaminopentan-dihydrochloride
Add. Screen II Nr.:14	30% 1,8 Diaminooctane
Add. Screen II Nr.:17	0.1M Hexaaminocobalt-trichloride
Add. Screen III Nr.:02	1.0M Cesium-chloride

Add. Screen III Nr.:04	1.0M Lihium-chloride
Add. Screen III Nr.:06	0.5M Sodium-flouride
Add. Screen III Nr.:16	40% Acetonitrile
Add. Screen III Nr.:18	40% n-Propanol
Add. Screen III Nr.:19	5% Ethyl-acetate
Add. Screen III Nr.:20	40% Acetone
Add. Screen III Nr.:21	2,5% Dichlormethane
Add. Screen III Nr.:22	7% n-Butanol
Add. Screen III Nr.:24	0.1M 1,4 Dithio-DL-threitol

B. Data collection:

Data were measured at the beam line BW 6 of the Max-Planck-Society at DESY, Hamburg.

The crystals were shock cooled to 100 K; cryobuffer was crystallization buffer plus 20 – 30 % glycerol. 213 frames with delta phi=0.25 degrees were collected with a MAR CCD detector, at a crystal detector distance of 120mm and a wavelength of 1.072Å.

Crystals are of a tetragonal space group with unit cell dimensions a=b=86.0 Å and c=112.0 Å. The cell dimensions of different crystals vary (for a and b between 85 and 87Å, for c between 97 and 113). Extinctions indicate the space group P42212 which was confirmed by molecular replacement.

Table II: Crystallization conditions for Tie-2/inhibitor complexes.

Condition	Tie-2 802-1124 D964N	Tie-2 802-1124 (diphosphorylated)
Protein concentration	2.5 mg/mL optimal range 1.5 – 4 mg/mL limits 1.0 – 5.0 mg/mL	5 mg/mL optimal range 2.5 – 10 mg/mL
Buffer concentration	100 mM MES optimal range 50–250 mM Limits 20–300 mM	100 mM HEPES optimal Range 50-150 mM Limits 20-300 mM
pH	6.5 optimal range 5.5 – 7.5	7.5 optimal range 7.0 – 7.7 limits 6.5 – 8.0
Buffer Identity	Buffers capable of buffering in a similar pH range expected to give similar results	(same)
Precipitant	$(NH_4)_2SO_4$ Range 1.0 – 1.5 M Limits 0.7 – 1.8 M	10% PEG 6000 optimal conc. range 5-15% conc. limits 1 – 20% MW range 4000 – 8000 MW limits may be much wide
Additive parameters	5% 1,4-dioxane optimal range 0 – 10% (higher concentrations etch the plastic vessel in which the experiment is done; higher concentrations may be possible in a resistant vessel) 1,3-dioxane, similar molecules, or mixtures in various ratios should also give similar results	5% MPD (2-Me-2,4-pentanedi optimal range 0 – 10%

Additive identities	Examples which have been successfully added: 1,5-diaminopentane Glycerol (1-10%) Ethylene glycol (1-10%) Spermidine (10 – 300 mM) Combinations, in varying ratios, may give similar results	(same)
Drop volumes and ratios	2 μL protein + 2 μL well solution optimal Total volume range: up to 200 μL, assuming a sitting geometry for larger volumes Volume Ratio range: 1 part protein to 0.5 – 2.0 parts well solution	(same)
Well volume (for 4 μL crystallization drop)	Range 500 – 1000 μL Limits 250 – large volume (limited by the distance between the drop and the surface of the well solution allowed by the vessel geometry, see below)	(same)
Drop – well solution distance	2 cm optimal Range 1-4 cm Limits: 0.1 cm - 5 cm	(same)
Temperature	room temp optimal (22 – 25 °C) limits 17 – 30 °C	(same)
Ligands	ADP/Mg^{2+} and analogs Inhibitors: inhibitors I-IV, analogs Expect similar results from ligands that bind reversibly under crystallization conditions with K_d values < 1 mM	(same)

Constructs	Variants in amino acid sequence that crystallize in the same space group and unit cell should be considered equivalent Additional constructs would include deletion of unstructured termini as determined by crystal structure of this construct. For example, deletion of the C-terminal 24 residues (leaving 802-1100 has been prepared, which is likely to yield similar results	(same)
Posttranslational modification	Variants in posttranslational modification that crystallize in the same space group and unit cell should be considered equivalent	2 phosphate forms have been crystallized. This protein cont one phosphate on either Y897 Y899 and one on one of five T residues, at amino acids 1012, 1024, 1040, and 1048 Other phosphorylated forms m give similar results. A single phosphate species has observed in which the phospha on either Y897 or Y899 has al: been isolated. In addition, 3 and 4 phosphate species have been isolated whi may crystallize.
Space group	C222(1)	P2(1)2(1)2(1)
Unit cell	a = 75.195 Å, b = 116.287 Å, c = 95.060 Å Variations of ± 2% should be considered equivalent Angles: a = b = c = 90° Observed variations of ± 1% should be considered equivalent	a = 54.320 Å, b = 75.872 Å, c 78.143 Å Variations of ± 2% should be considered equivalent Angles: a = b = c = 90° Observed variations of ± 1% should be considered equivale

Other crystallization tricks that should give at least equivalent results	Low gravity Temperature oscillations Presence of cryoprotectant (15-25% glycerol added before data collection) Variations in crystallization tray geometry Data collection temperature (range: minus 180 to plus 25 °C)	(same)

REFERENCES:

Brunger, A.T., Adams, P. D., Clore, G. M., DeLano, W. L. Gros, P. Grosse-Kunstleve, R. W., Jiang, J-S., Kuszewski, J., Nigels, M., Pannu, N. S., Read, R. J., Rice, L. M., Simonson, T., and Warren, G. L.. (1998) *Acta Cryst., D54,* 905-921.

Collaborative Computational Project, Number 4 (1994) The CCP4 Suite: Programs for Protein Crystallography. *Acta Crys.t D50,* 760-763.

Jones, A.T and Kjeldgaard, M. (1997) Methods in Enzymology 277, 173-208.

Kleywegt G. J. and Jones, T.A. (1997) Methods in Enzymology 277, 525-545.

Kleywegt G. J., (1995) ESF/CCP4 Newsletter 31, 45-50.

Minor, W. XDISPLAYF program, Purdue University (1993)

Navaza, J. (1994) *Acta Cryst. A50,* 157-163.

Example 3: *In Vitro* Potency Test of Tie-2 Inhibitors

The *in vitro* potency of compounds in inhibiting these protein kinases may be determined by the procedures detailed below.

The potency of compounds can be determined by the amount of inhibition of the phosphorylation of an exogenous substrate (e.g., synthetic peptide (Z. Songyang *et al., Nature.* 373:536-539) by a test compound relative to control.

Human Tie-2 Kinase Production and Purification

The coding sequence for the human Tie-2 intra-cellular domain (aa775-1124) was generated through PCR using cDNAs isolated from human placenta as a template. A poly-His_6 sequence was introduced at the N-terminus and this construct was cloned into transfection vector pVL 1939 at the Xba 1 and Not 1 site. Recombinant BV was generated through co-transfection using the BaculoGold Transfection reagent (PharMingen). Recombinant BV was plaque purified and verified through Western analysis. For protein production, SF-9 insect cells were grown in SF-900-II medium at 2 x 106/ml, and were infected at MOI of 0.5. Purification of the His-tagged kinase used in screening was analogous to that described for KDR.

EGFR Tyrosine Kinase Source

EGFR was purchased from Sigma (Cat # E-3641; 500 units/50 l) and the EGF ligand was acquired from Oncogene Research Products/Calbiochem (Cat # PF011-100).

Enzyme Linked Immunosorbent Assay (ELISA) For PTKs

Enzyme linked immunosorbent assays (ELISA) were used to detect and measure the presence of tyrosine kinase activity. The ELISA were conducted according to known protocols which are described in, for example, Voller, *et al.*, 1980, "Enzyme-Linked Immunosorbent Assay," In: *Manual of Clinical Immunology, 2d ed.*, edited by Rose and Friedman, pp 359-371 Am. Soc. of Microbiology, Washington, D.C.

The disclosed protocol was adapted for determining activity with respect to a specific PTK. For example, preferred protocols for conducting the ELISA experiments is provided below. Adaptation of these protocols for determining a

compound's activity for other members of the receptor PTK family, as well as non-receptor tyrosine kinases, are well within the abilities of those skilled in the art. For purposes of determining inhibitor selectivity, a universal PTK substrate (e.g., random copolymer of poly(Glu_4 Tyr), 20,000-50,000 MW) was employed together with ATP (typically 5 μM) at concentrations approximately twice the apparent Km in the assay.

The following procedure was used to assay the inhibitory effect of compounds of this invention on Tie-2 tyrosine kinase activity:

Buffers and Solutions:

PGTPoly (Glu,Tyr) 4:1

Store powder at -20°C. Dissolve powder in phosphate buffered saline (PBS) for 50mg/ml solution. Store 1ml aliquots at -20°C. When making plates dilute to 250 g/ml in Gibco PBS.

Reaction Buffer: 100mM Hepes, 20mM $MgCl_2$, 4mM $MnCl_2$, 5mM DTT, 0.02%BSA, 200μM $NaVO_4$, pH 7.10

ATP: Store aliquots of 100mM at -20°C. Dilute to 20μM in water

Washing Buffer: PBS with 0.1% Tween 20

Antibody Diluting Buffer: 0.1% bovine serum albumin (BSA) in PBS

TMB Substrate: mix TMB substrate and Peroxide solutions 9:1 just before use or use K-Blue Substrate from Neogen

Stop Solution: 1M Phosphoric Acid

Procedure

1. Plate Preparation:

Dilute PGT stock (50mg/ml, frozen) in PBS to a 250μg/ml. Add 125μl per well of Corning modified flat bottom high affinity ELISA plates (Corning #25805-96). Add 125μl PBS to blank wells. Cover with sealing tape and incubate overnight 37°C. Wash 1x with 250μl washing buffer and dry for about 2hrs in 37°C dry incubator. Store coated plates in sealed bag at 4°C until used.

2. Tyrosine Kinase Reaction:

-Prepare inhibitor solutions at a 4x concentration in 20% DMSO in water.

-Prepare reaction buffer

-Prepare enzyme solution so that desired units are in 50µl, e.g. for KDR make to 1 ng/ l for a total of 50ng per well in the reactions. Store on ice.

-Make 4x ATP solution to 20µM from 100mM stock in water. Store on ice

-Add 50µl of the enzyme solution per well (typically 5-50 ng enzyme/well depending on the specific activity of the kinase)

-Add 25µl 4x inhibitor

-Add 25µl 4x ATP for inhibitor assay

-Incubate for 10 minutes at room temperature

-Stop reaction by adding 50µl 0.05N HCl per well

-Wash plate

**Final Concentrations for Reaction: 5µM ATP, 5% DMSO

3. Antibody Binding

-Dilute 1mg/ml aliquot of PY20-HRP (Pierce) antibody (a phosphotyrosine antibody) to 50ng/ml in 0.1% BSA in PBS by a 2 step dilution (100x, then 200x)

-Add 100µl Ab per well. Incubate 1 hr at room temp. Incubate 1 hr at 4C.

-Wash 4x plate

4. Color reaction

-Prepare TMB substrate and add 100µl per well

-Monitor OD at 650nm until 0.6 is reached

-Stop with 1M Phosphoric acid. Shake on plate reader.

-Read OD immediately at 450nm

Optimal incubation times and enzyme reaction conditions vary slightly with enzyme preparations and are determined empirically for each lot.

Example 4: Cellular Assay for Determining the Potency of Tie-2 Inhibitors

The following cellular assay can be used to determine the potency of a Tie-2 inhibitor.

"NIH-3T3/hTEK Cell line:

A retroviral expression vector containing the full length Tie-2 cDNA, LNCX6 h-TEK, was kindly provided to us by Dr. Kevin Peters. A tumorigenic subline of NIH 3T3 cells was transfected with 10 ìg of LNCX6 h-TEK by calcium phosphate precipitation method and selected with 400 ìg/ml neomycin. Individual clones were isolated and analyzed for the presence of Tie-2 protein by Western blotting. Maximum expression of Tie-2 was observed in clone #67. Expression of Angiopoietin 1 message has been shown using PCR and an autocrine loop is revealed in the presence of vanadate

Cellular Tie-2 assay:

Tie-2 cellular autophosphorylation was measured using the NIH-3T3/hTEK (hTEK) cell line. Cells were seeded in 96 well plates overnight. The media was removed and cells treated with inhibitor for 20 minutes and phosphotase inhibitor $NaVO_3$ (2mM) for 15 more minutes. Cells were lysed with RIPA buffer and lysates were immunoprecipitated using a specific a-Tie-2 monoclonal antibody (KP33, provided by Dr. Kevin Peters) and the IP'd protein run on SDS PAGE. The phosphotyrosine level on Tie2 protein were then determined by a-phosphotyrosine antibodies (4G10, Upstate Biotechnology) on Western blots. Films were scanned and % inhibition as compared to untreated control was determined."

EQUIVALENTS

While this invention has been particularly shown and described with references to preferred embodiments thereof, it will be understood by those skilled in the art that various changes in form and details may be made therein without departing from the scope of the invention encompassed by the appended claims.

CLAIMS

What is claimed is:

1. A crystalline polypeptide, said polypeptide comprising the catalytic domain of a Tie-2 protein.

2. The crystalline polypeptide of Claim 1 wherein the polypeptide comprises the catalytic domain of human Tie-2.

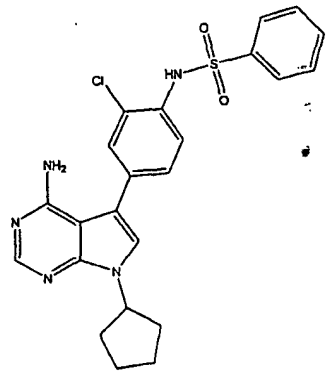
3. A crystalline polypeptide-ligand complex, said polypeptide comprising the catalytic domain of a Tie-2 protein.

4. The crystalline polypeptide/ligand complex of Claim 3 wherein the polypeptide comprises the catalytic domain of a mammalian Tie-2.

5. The crystalline polypeptide/ligand complex of Claim 4 wherein the mammalian Tie-2 protein is human Tie-2.

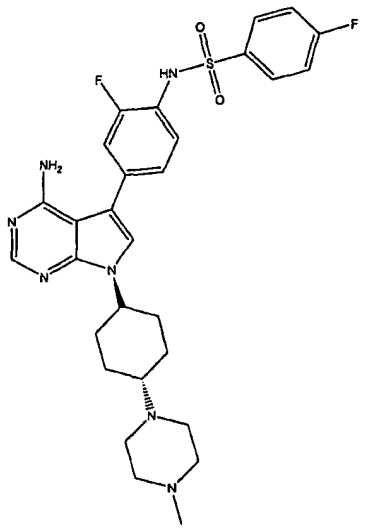
6. The crystalline polypeptide/ligand complex of Claim 5 wherein the polypeptide comprises amino acids 802-1124 of SEQ ID NO: 1.

7. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:



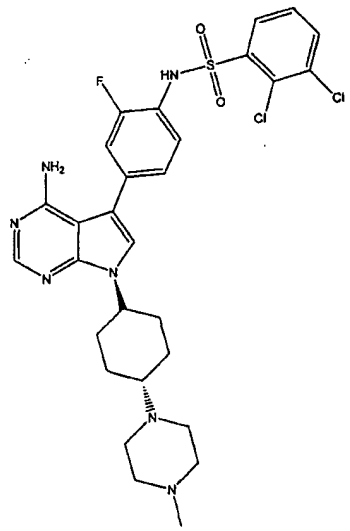
8. The crystalline polypeptide/ligand complex of Claim 7 having unit cell parameters a is about 96 Å, b is about 118 Å, c is about 78 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

9. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:



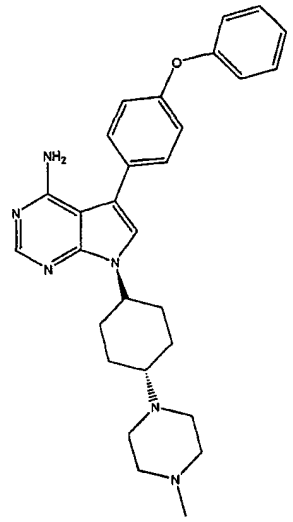
10. The crystalline polypeptide/ligand complex of Claim 9 having unit cell parameters a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

11. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:



12. The crystalline polypeptide/ligand complex of Claim 11 having unit cell parameters a and b are about 86.0 Å, and c is about 112.0 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

13. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:



14. The crystalline polypeptide/ligand complex of Claim 13 having unit cell parameters a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

15. A method of determining the three dimensional structure of a first polypeptide comprising the catalytic domain of a Tie-2 protein, said method comprising the steps of:

(a) obtaining a crystal of the first polypeptide comprising the catalytic domain of Tie-2;

(b) obtaining x-ray diffraction data for said crystal; and

(c) solving the crystal structure of said crystal using the atomic coordinates of a second polypeptide and said x-ray diffraction data, said second polypeptide comprising the catalytic domain of a Tie-2 protein.

16. The method of Claim 15 wherein the crystal of the first polypeptide comprises the first polypeptide complexed with a ligand.

17. The method of Claim 15 wherein the first polypeptide comprises the catalytic domain of a mammalian Tie-2 protein.

18. The method of Claim 17 wherein the first polypeptide and the second polypeptide, independently, comprise the catalytic domain of a human Tie-2 protein.

19. The method of Claim 18, wherein the first polypeptide comprises the catalytic domain of wild type human Tie-2 and the second polypeptide comprises the catalytic domain of wild type human Tie-2.

20. The method of Claim 19, wherein the first polypeptide comprises the catalytic domain of wild type human Tie-2.

21. A method of identifying a compound which is an inhibitor of a Tie-2 protein, said method comprising the steps of

(a) obtaining the atomic coordinates of a crystal of a polypeptide comprising the catalytic domain of a Tie-2 protein;

(b) using said atomic coordinates to define the active subsites of Tie-2; and

(c) identifying a compound which binds to the one or more active subsite; wherein the compound which bind to the active subsite or sites is an inhibitor of a Tie-2 protein.

22. The method of Claim 21, further comprising the step of

(d) assessing the ability of the compound identified in step (c) to inhibit Tie-2.

23. The method of Claim 21 wherein the Tie-2 protein is a mammalian protein.

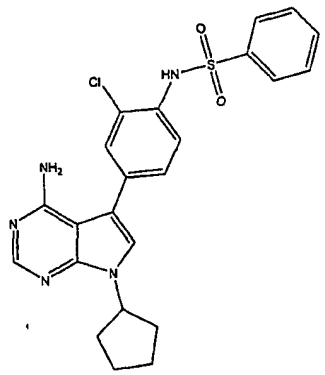
24. The method of Claim 22 wherein the Tie-2 protein is a human protein.

25. The method of Claim 24, wherein the Tie-2 protein is wild type human Tie-2.

26. The method of Claim 21 wherein said crystal further comprises a ligand bound to said catalytic domain.

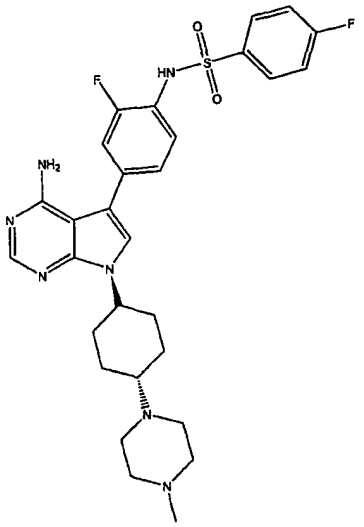
27. The method of Claim 24 wherein the polypeptide comprises amino acids 802-1124 of SEQ ID NO: 1.

28. The method of Claim 24, wherein the ligand is of the formula:



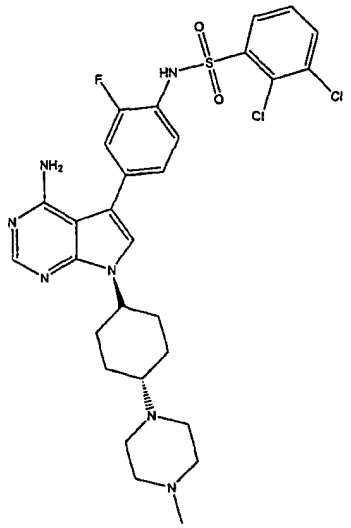
29. The method of Claim 28, wherein the crystal has unit cell parameters wherein a is about 96 Å, b is about 118 Å, c is about 78 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

30. The method of Claim 24,wherein the ligand is of the formula:



31. The method of Claim 30, wherein the crystal has unit cell parameters wherein a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

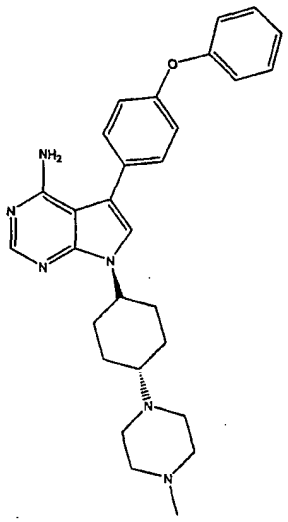
32. The method of Claim 24, wherein the ligand is of the formula:



33. The method of Claim 32, wherein the crystal has unit cell parameters wherein

a and b are about 86.0 Å, and c is about 112.0 Å and $\alpha = \beta = \gamma = 90°$.

34. The method of Claim 24, wherein the ligand is of the formula:



35. The method of Claim 34, wherein the crystal has unit cell parameters wherein a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90°$.

36. A method of identifying a compound which is a potential inhibitor of a Tie-2 protein, said method comprising the step of designing a compound that will interact with one or more subsites in the catalytic domain of the Tie-2 protein, based upon the crystal structure coordinates of a polypeptide comprising the catalytic domain; wherein said compound is identified as a potential inhibitor of the Tie-2 protein.

37. The method of Claim 36 wherein the Tie-2 protein is a mammalian Tie-2 protein.

38. The method of Claim 37 wherein the Tie-2 protein is a human Tie-2 protein.

39. The method of Claim 38, wherein the Tie-2 protein is wild type human Tie-2.

40. The method of Claim 39 wherein the polypeptide comprises amino acids 802-1124 of SEQ ID NO: 1.

41. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 3.

42. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 4.

43. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 5.

44. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 6.

45. The method of Claim 38 wherein the compound interacts with one or more of subsites 1 to 9.

46. The method of Claim 45 wherein the compound interacts with two or more of subsites 1 to 9.

47. The method of Claim 46 wherein the compound interacts with three or more of subsites 1 to 9.

48. The method of Claim 46 wherein the compound interacts with a set of subsites comprising subsite 1 and subsite 2.

49. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2 and subsite 3.

50. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2 and subsite 8.

51. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3 and subsite 8.

52. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 4 and subsite 5.

53. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 7 and subsite 8.

54. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 7 and subsite 8.

55. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 7 and subsite 8.

56. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 4, subsite 6 and subsite 8.

57. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 4, subsite 6 and subsite 8.

58. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 4, subsite 6 and subsite 8.

59. A Tie-2 inhibitor comprising two or more of the following:

(a) a hydrogen bond donor positioned to interact with Glu 903 of human Tie-2;

(b) a hydrogen bond acceptor positioned to interact with Ala 905 of human Tie-2;

(c) a hydrogen bond donor positioned to interact with Ala 905 of human Tie-2;

(d) a hydrophobic moiety positioned to interact with one or more of Ile 830, Val 838, Ala 853, Ile 886, Ile 902, Tyr 904, Ala 905 and Leu 971 of human Tie-2;

(e) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 912 of human Tie-2;

(f) a hydrogen bond donor or hydrogen bond acceptor postioned to interact with Asn 909 of human Tie-2;

(g) a hydrophobic moiety positioned to interact with one or more of Val 838, Lys 855, Ile 886, Ile 902, Leu 971 and Ala 981 of human Tie-2;

(h) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 855 of human Tie-2;

(i) a hydrogen bond acceptor positioned to interact with Asp 982 of human Tie-2;

(j) a hydrogen bond acceptor positioned to interact with Phe 983 of human Tie-2;

(k) a hydrophobic moiety positioned to interact with one or more of Leu 873, Leu 876, Ile 885, Ile 886, Leu 888, Leu 900, Ile 902, Ala 981 and Phe 983 of human Tie-2;

(l) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 982 of human Tie-2;

(m) a hydrogen bond donor positioned to interact with Ile 886 of human Tie-2;

(n) a hydrogen bond donor positioned to interact with Leu 768 of human Tie-2;

(o) a hydrogen bond acceptor positioned to interact with Gly 831 of human Tie-2;

(p) a hydrogen bond donor or positively charged functional group

positioned to interact with Glu 832 of human Tie-2;

(q) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 840 of human Tie-2;

(r) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 916 of human Tie-2;

(s) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Arg 968 of human Tie-2;

(t) a hydrogen bond donor positioned to interact with Arg 968 of human Tie-2.

60. The Tie-2 inhibitor of Claim 59 comprising (b) and (d).

61. The Tie-2 inhibitor of Claim 59 comprising (d) and at least one of (a), (b) and (c).

62. The Tie-2 inhibitor of Claim 59 comprising (d) and at least two of (a), (b) and (c).

63. The Tie-2 inhibitor of Claim 62 further comprising at least one of (e) and (f).

64. The Tie-2 inhibitor of Claim 62 further comprising (g).

65. The Tie-2 inhibitor of Claim 63 further comprising (g).

66. The Tie-2 inhibitor of Claim 64 further comprising (k).

67. The Tie-2 inhibitor of Claim 65 further comprising (k).

68. The Tie-2 inhibitor of Claim 62 further comprising at least one of (i) and (j).

69. The Tie-2 inhibitor of Claim 63 further comprising at least one of (i) and (j).

70. The Tie-2 inhibitor of Claim 66 further comprising at least one of (i) and (j).

71. The Tie-2 inhibitor of Claim 67 further comprising at least one of (i) and (j).

72. The Tie-2 inhibitor of Claim 59, wherein the inhibitor has a Ki of at least about 1 mM.

73. The Tie-2 inhibitor of Claim 59, wherein the inhibitor has a Ki of at least about 100 μM.

74. The Tie-2 inhibitor of Claim 59, wherein the inhibitor has a Ki of at least about 10 μM.

75. The Tie-2 inhibitor of Claim 59, wherein the inhibitor selectively binds Tie-2 receptors.

76. A method of treating a Tie-2 dependent condition in a patient comprising the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor of Claim 59.

77. The method of Claim 76 wherein the patient is a human.

78. The method of Claim 76 wherein the Tie-2 dependent condition is characterized by excessive vascular proliferation.

79. The method of Claim 78 wherein the Tie-2 dependent condition is a hyperproliferative disorder, cancer, a cardiovascular condition, an ocular condition, von Hippel Lindau disease, pemphigoid, psoriasis, Paget's disease, polycystic kidney disease, fibrosis, sarcoidosis, cirrhosis, thyroiditis, Osler-Weber-Rendu disease, chronic inflammation, synovitis, inflammatory bowel disease, Crohn's disease, rheumatoid arthritis, osteoarthritis, psoriatic arthritis,

an ulcer or sepsis.

80. The method of Claim 79, wherein the condition is a cancer selected from the group consisting of solid tumor, a sarcoma, fibrosarcoma, osteoma, melanoma, retinoblastoma, a rhabdomyosarcoma, glioblastoma, neuroblastoma, teratocarcinoma, an hematopoietic malignancy, malignant ascites, Kaposi's sarcoma, Hodgkin's disease, lymphoma, myeloma and leukemia.

81. The method of Claim 79 wherein the condition is a cardiovascular condition selected from the group consisting of atherosclerosis, restenosis, ischemia/reperfusion injury, chronic occlusive pulmonary disease, vascular occlusion, carotid obstructive disease, Crow-Fukase (POEMS) syndrome, anemia, ischemia, infarct, and vascular leakage disorders.

82. The method of Claim 79 wherein the condition is an ocular condition selected from the group consisting of ocular or macular edema, ocular neovascular disease, scleritis, radial keratotomy, uveitis, vitritis, myopia, optic pits, chronic retinal detachment, post-laser treatment complications, conjunctivitis, Stargardt's disease, Eales disease, retinopathy, macular degeneration and microangiopathy.

83. The method of Claim 76, wherein the disorder involves aberrant endothelial-periendothelial interactions.

84. A method of decreasing fertility in a patient comprising the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor of Claim 59.

85. A method of promoting angiogenesis or vasculogenesis in a patient comprising the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor of Claim 59.

86. The method of Claim 85, wherein the Tie-2 inhibitor is administered in combination with a pro-angiogenic growth factor.

87. A method of determining the three dimensional structure of a polypeptide comprising the catalytic domain of a Tie-2 protein, said method comprising the steps of:

(a) obtaining a crystal of the polypeptide comprising the catalytic domain of Tie-2;

(b) obtaining x-ray diffraction data for said crystal; and

(c) solving the crystal structure of said crystal.

88. A crystalline polypeptide, said polypeptide comprising a sequence having 80% homology with the catalytic domain of a Tie-2 protein.

MDSLASLVLC GVSLLLSGTV EGAMDLILIN SLPLVSDAET SLTCIASGWR PHEPITIGRD
FEALMNQHQD PLEVTQDVTR EWAKKVVWKR EKASKINGAY FCEGRVRGEA IRIRTMKMRQ
QASFLPATLT MTVDKGDNVN ISFKKVLIKE EDAVIYKNGS FIHSVPRHEV PDILEVHLPH
AQPQDAGVYS ARYIGGNLFT SAFTRLIVRR CEAQKWGPEC NHLCTACMNN GVCHEDTGEC
ICPPGFMGRT CEKACELHTF GRTCKERCSG QEGCKSYVFC LPDPYGCSCA TGWKGLQCNE
ACHPGFYGPD CKLRCSCNNG EMCDRFQGCL CSPGWQGLQC EREGIPRMTP KIVDLPDHIE
VNSGKFNPIC KASGWPLPTN EEMTLVKPDG TVLHPKDFNH TDHFSVAIFT IHRILPPDSG
VWVCSVNTVA GMVEKPFNIS VKVLPKPLNA PNVIDTGHNF AVINISSEPY FGDGPIKSKK
LLYKPVNHYE AWQHIQVTNE IVTLNYLEPR TEYELCVQLV RRGEGGEGHP GPVRRFTTAS
IGLPPPRGLN LLPKSQTTLN LTWQPIFPSS EDDFYVEVER RSVQKSDQQN IKVPGNLTSV
LLNNLHPREQ YVVRARVNTK AQGEWSEDLT AWTLSDILPP QPENIKISNI THSSAVISWT
ILDGYSISSI TIRYKVQGKN EDQHVDVKIK NATIIQYQLK GLEPETAYQV DIFAENNIGS
SNPAFSHELV TLPESQAPAD LGGGKMLLIA ILGSAGMTCL TVLLAFLIIL QLKRANVQRR
MAQAFQNVRE EPAVQFNSGT LALNRKVKNN PDPTIYPVLD WNDIKFQDVI GEGNFGQVLK
ARIKKDGLRM DAAIKRMKEY ASKDDHRDFA GELEVLCKLG HHPNIINLLG ACEHRGYLYL
AIEYAPHGNL LDFLRKSRVL ETDPAFAIAN STASTLSSQQ LLHFAADVAR GMDYLSQKQF
IHRDLAARNI LVGENYVAKI ADFGLSRGQE VYVKKTMGRL PVRWMAIESL NYSVYTTNSD
VWSYGVLLWE IVSLGGTPYC GMTCAELYEK LPQGYRLEKP LNCDDEVYDL MRQCWREKPY
ERPSFAQILV SLNRMLEERK TYVNTTLYEK FTYAGIDCSA EEAA

FIG. 1

ALNRKVKNN PDPTIYPVLD WNDIKFQDVI GEGNFGQVLK
ARIKKDGLRM DAAIKRMKEY ASKDDHRDFA GELEVLCKLG
HHPNIINLLG ACEHRGYLYL AIEYAPHGNL LDFLRKSRVL
ETDPAFAIAN STASTLSSQQ LLHFAADVAR GMDYLSQKQF
IHRNLAARNI LVGENYVAKI ADFGLSRGQE VYVKKTMGRL
PVRWMAIESL NYSVYTTNSD VWSYGVLLWE IVSLGGTPYC
GMTCAELYEK LPQGYRLEKP LNCDDEVYDL MRQCWREKPY
ERPSFAQILV SLNRMLEERK TYVNTTLYEK FTYAGIDCSA
EEAA

FIG. 2

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CRYST1   95.604  117.589   78.214  90.00  90.00  90.00
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.010460  0.000000  0.000000        0.00000
SCALE2      0.000000  0.008504  0.000000        0.00000
SCALE3      0.000000  0.000000  0.012785        0.00000
ATOM      1  CB  VAL   818       5.159  51.390 -17.822  1.00 65.41    6
ATOM      2  C   VAL   818       3.553  51.091 -15.926  1.00 99.70    6
ATOM      3  O   VAL   818       2.603  51.682 -16.444  1.00 99.70    8
ATOM      4  N   VAL   818       4.074  49.203 -17.428  1.00 99.70    7
ATOM      5  CA  VAL   818       4.628  50.419 -16.774  1.00 99.70    6
ATOM      6  N   LEU   819       3.729  50.991 -14.616  1.00100.00    7
ATOM      7  CA  LEU   819       2.912  51.555 -13.639  1.00100.00    6
ATOM      8  CB  LEU   819       3.310  51.175 -12.250  1.00 77.77    6
ATOM      9  CG  LEU   819       2.625  51.796 -11.045  1.00 67.90    6
ATOM     10  CD1 LEU   819       1.161  51.416 -11.022  1.00 67.90    6
ATOM     11  CD2 LEU   819       3.336  51.313  -9.810  1.00 67.90    6
ATOM     12  C   LEU   819       2.607  53.076 -13.729  1.00100.00    6
ATOM     13  O   LEU   819       3.568  53.838 -13.899  1.00100.00    8
ATOM     14  N   ASP   820       1.351  53.507 -13.602  1.00100.00    7
ATOM     15  CA  ASP   820       0.990  54.928 -13.659  1.00100.00    6
ATOM     16  CB  ASP   820      -0.505  55.084 -13.929  1.00100.00    6
ATOM     17  CG  ASP   820      -0.910  56.525 -14.140  1.00100.00    6
ATOM     18  OD1 ASP   820      -2.054  56.874 -13.785  1.00100.00    8
ATOM     19  OD2 ASP   820      -0.087  57.303 -14.663  1.00100.00    8
ATOM     20  C   ASP   820       1.314  55.593 -12.329  1.00100.00    6
ATOM     21  O   ASP   820       0.786  55.200 -11.290  1.00100.00    8
ATOM     22  N   TRP   821       2.171  56.605 -12.361  1.00100.00    7
ATOM     23  CA  TRP   821       2.558  57.278 -11.132  1.00100.00    6
ATOM     24  CB  TRP   821       3.291  58.582 -11.458  1.00 96.30    6
ATOM     25  CG  TRP   821       3.985  59.118 -10.263  1.00 96.04    6
ATOM     26  CD2 TRP   821       3.369  59.782  -9.149  1.00 96.04    6
ATOM     27  CE2 TRP   821       4.371  59.991  -8.185  1.00 96.04    6
ATOM     28  CE3 TRP   821       2.061  60.200  -8.869  1.00 96.04    6
ATOM     29  CD1 TRP   821       5.302  58.974  -9.938  1.00 96.04    6
ATOM     30  NE1 TRP   821       5.545  59.494  -8.689  1.00 96.04    7
ATOM     31  CZ2 TRP   821       4.106  60.614  -6.976  1.00 96.04    6
ATOM     32  CZ3 TRP   821       1.803  60.816  -7.657  1.00 96.04    6
ATOM     33  CH2 TRP   821       2.824  61.007  -6.733  1.00 96.04    6
ATOM     34  C   TRP   821       1.355  57.543 -10.207  1.00100.00    6
ATOM     35  O   TRP   821       1.462  57.434  -8.983  1.00100.00    8
ATOM     36  N   ASN   822       0.207  57.853 -10.801  1.00 78.55    7
ATOM     37  CA  ASN   822      -1.018  58.149 -10.061  1.00 78.55    6
ATOM     38  CB  ASN   822      -2.158  58.380 -11.037  1.00100.00    6
ATOM     39  CG  ASN   822      -3.126  59.416 -10.546  1.00100.00    6
ATOM     40  OD1 ASN   822      -3.508  60.321 -11.291  1.00100.00    8
ATOM     41  ND2 ASN   822      -3.536  59.303  -9.286  1.00100.00    7
ATOM     42  C   ASN   822      -1.453  57.094  -9.048  1.00 78.55    6
ATOM     43  O   ASN   822      -1.451  57.340  -7.842  1.00 78.55    8
ATOM     44  N   ASP   823      -1.854  55.933  -9.554  1.00 95.03    7
ATOM     45  CA  ASP   823      -2.308  54.841  -8.704  1.00 95.03    6
ATOM     46  CB  ASP   823      -2.991  53.775  -9.562  1.00 65.89    6
ATOM     47  C   ASP   823      -1.158  54.218  -7.916  1.00 95.03    6
```

FIG. 3A

ATOM	48	O	ASP	823	-0.967	53.008	-7.949	1.00 95.03	8
ATOM	49	N	ILE	824	-0.384	55.043	-7.221	1.00 88.67	7
ATOM	50	CA	ILE	824	0.729	54.531	-6.426	1.00 88.67	6
ATOM	51	CB	ILE	824	2.112	54.819	-7.082	1.00 53.67	6
ATOM	52	CG2	ILE	824	3.202	54.080	-6.326	1.00 56.64	6
ATOM	53	CG1	ILE	824	2.161	54.314	-8.526	1.00 56.64	6
ATOM	54	CD1	ILE	824	3.503	54.615	-9.196	1.00 56.64	6
ATOM	55	C	ILE	824	0.701	55.176	-5.041	1.00 88.67	6
ATOM	56	O	ILE	824	1.617	55.912	-4.665	1.00 88.67	8
ATOM	57	N	LYS	825	-0.361	54.889	-4.292	1.00 65.97	7
ATOM	58	CA	LYS	825	-0.552	55.426	-2.947	1.00 65.97	6
ATOM	59	CB	LYS	825	-1.917	54.995	-2.406	1.00 30.30	6
ATOM	60	C	LYS	825	0.544	55.003	-1.973	1.00 65.97	6
ATOM	61	O	LYS	825	0.502	53.909	-1.401	1.00 65.97	8
ATOM	62	N	PHE	826	1.526	55.879	-1.788	1.00 96.52	7
ATOM	63	CA	PHE	826	2.632	55.608	-0.878	1.00 96.52	6
ATOM	64	CB	PHE	826	3.784	56.586	-1.112	1.00 96.59	6
ATOM	65	CG	PHE	826	4.397	56.474	-2.463	1.00100.00	6
ATOM	66	CD1	PHE	826	3.989	57.310	-3.489	1.00100.00	6
ATOM	67	CD2	PHE	826	5.351	55.500	-2.726	1.00100.00	6
ATOM	68	CE1	PHE	826	4.518	57.181	-4.764	1.00100.00	6
ATOM	69	CE2	PHE	826	5.888	55.358	-4.001	1.00100.00	6
ATOM	70	CZ	PHE	826	5.469	56.202	-5.023	1.00100.00	6
ATOM	71	C	PHE	826	2.158	55.727	0.565	1.00 96.52	6
ATOM	72	O	PHE	826	1.746	56.794	0.991	1.00 96.52	8
ATOM	73	N	GLN	827	2.247	54.651	1.332	1.00100.00	7
ATOM	74	CA	GLN	827	1.769	54.708	2.698	1.00100.00	6
ATOM	75	CB	GLN	827	0.886	53.484	2.937	1.00100.00	6
ATOM	76	CG	GLN	827	-0.252	53.407	1.903	1.00100.00	6
ATOM	77	CD	GLN	827	-1.539	52.860	2.488	1.00100.00	6
ATOM	78	OE1	GLN	827	-1.553	51.771	3.060	1.00100.00	8
ATOM	79	NE2	GLN	827	-2.633	53.615	2.349	1.00100.00	7
ATOM	80	C	GLN	827	2.840	54.886	3.781	1.00100.00	6
ATOM	81	O	GLN	827	2.892	55.942	4.395	1.00100.00	8
ATOM	82	N	ASP	828	3.696	53.894	4.015	1.00 99.72	7
ATOM	83	CA	ASP	828	4.713	54.034	5.064	1.00 99.72	6
ATOM	84	CB	ASP	828	4.144	53.510	6.388	1.00 87.03	6
ATOM	85	CG	ASP	828	5.121	53.627	7.533	1.00 84.60	6
ATOM	86	OD1	ASP	828	5.870	54.617	7.572	1.00 84.60	8
ATOM	87	OD2	ASP	828	5.128	52.740	8.406	1.00 84.60	8
ATOM	88	C	ASP	828	6.003	53.286	4.720	1.00 99.72	6
ATOM	89	O	ASP	828	5.961	52.262	4.034	1.00 99.72	8
ATOM	90	N	VAL	829	7.154	53.772	5.178	1.00 85.45	7
ATOM	91	CA	VAL	829	8.408	53.075	4.863	1.00 85.45	6
ATOM	92	CB	VAL	829	9.606	53.874	5.391	1.00 51.35	6
ATOM	93	C	VAL	829	8.460	51.633	5.402	1.00 85.45	6
ATOM	94	O	VAL	829	8.437	51.418	6.615	1.00 85.45	8
ATOM	95	N	ILE	830	8.538	50.663	4.488	1.00100.00	7
ATOM	96	CA	ILE	830	8.598	49.244	4.852	1.00100.00	6
ATOM	97	CB	ILE	830	8.745	48.326	3.602	1.00100.00	6
ATOM	98	CG2	ILE	830	9.458	47.031	3.973	1.00 81.07	6
ATOM	99	CG1	ILE	830	7.370	48.034	2.994	1.00 81.07	6
ATOM	100	CD1	ILE	830	6.385	47.414	3.969	1.00 81.07	6
ATOM	101	C	ILE	830	9.788	49.013	5.769	1.00100.00	6
ATOM	102	O	ILE	830	9.782	48.103	6.596	1.00100.00	8
ATOM	103	N	GLY	831	10.821	49.834	5.605	1.00 95.79	7
ATOM	104	CA	GLY	831	11.992	49.713	6.453	1.00 95.79	6

FIG. 3B

ATOM	105	C	GLY	831	13.352	49.743	5.806	1.00 95.79	6
ATOM	106	O	GLY	831	13.497	50.005	4.613	1.00 95.79	8
ATOM	107	N	GLU	832	14.357	49.480	6.630	1.00 99.78	7
ATOM	108	CA	GLU	832	15.760	49.427	6.231	1.00 99.78	6
ATOM	109	CB	GLU	832	16.055	48.055	5.602	1.00100.00	6
ATOM	110	CG	GLU	832	16.417	46.997	6.632	1.00100.00	6
ATOM	111	CD	GLU	832	17.103	47.598	7.859	1.00100.00	6
ATOM	112	OE1	GLU	832	16.380	48.153	8.721	1.00100.00	8
ATOM	113	OE2	GLU	832	18.352	47.535	7.943	1.00100.00	8
ATOM	114	C	GLU	832	16.376	50.502	5.339	1.00 99.78	6
ATOM	115	O	GLU	832	15.689	51.284	4.679	1.00 99.78	8
ATOM	116	N	GLY	833	17.708	50.501	5.333	1.00100.00	7
ATOM	117	CA	GLY	833	18.494	51.424	4.536	1.00100.00	6
ATOM	118	C	GLY	833	19.580	50.682	3.756	1.00100.00	6
ATOM	119	O	GLY	833	19.557	49.446	3.693	1.00100.00	8
ATOM	120	N	ASN	834	20.540	51.432	3.192	1.00100.00	7
ATOM	121	CA	ASN	834	21.643	50.854	2.407	1.00100.00	6
ATOM	122	CB	ASN	834	22.414	49.810	3.241	1.00100.00	6
ATOM	123	CG	ASN	834	23.700	49.360	2.579	1.00100.00	6
ATOM	124	OD1	ASN	834	23.727	49.066	1.387	1.00100.00	8
ATOM	125	ND2	ASN	834	24.778	49.302	3.354	1.00100.00	7
ATOM	126	C	ASN	834	21.094	50.179	1.149	1.00100.00	6
ATOM	127	O	ASN	834	20.299	49.228	1.240	1.00100.00	8
ATOM	128	N	PHE	835	21.519	50.650	-0.030	1.00100.00	7
ATOM	129	CA	PHE	835	21.056	50.117	-1.328	1.00100.00	6
ATOM	130	CB	PHE	835	22.041	49.061	-1.877	1.00100.00	6
ATOM	131	CG	PHE	835	23.383	49.629	-2.294	1.00100.00	6
ATOM	132	CD1	PHE	835	24.562	48.976	-1.954	1.00100.00	6
ATOM	133	CD2	PHE	835	23.465	50.835	-2.996	1.00100.00	6
ATOM	134	CE1	PHE	835	25.808	49.509	-2.291	1.00100.00	6
ATOM	135	CE2	PHE	835	24.706	51.380	-3.342	1.00100.00	6
ATOM	136	CZ	PHE	835	25.879	50.718	-2.987	1.00100.00	6
ATOM	137	C	PHE	835	19.641	49.519	-1.261	1.00100.00	6
ATOM	138	O	PHE	835	19.380	48.467	-1.841	1.00100.00	8
ATOM	139	N	GLY	836	18.748	50.228	-0.570	1.00100.00	7
ATOM	140	CA	GLY	836	17.369	49.813	-0.397	1.00100.00	6
ATOM	141	C	GLY	836	16.689	50.596	0.720	1.00100.00	6
ATOM	142	O	GLY	836	17.188	50.622	1.840	1.00100.00	8
ATOM	143	N	GLN	837	15.571	51.261	0.418	1.00100.00	7
ATOM	144	CA	GLN	837	14.831	52.043	1.420	1.00100.00	6
ATOM	145	CB	GLN	837	15.333	53.505	1.397	1.00100.00	6
ATOM	146	CG	GLN	837	14.344	54.609	1.081	1.00100.00	6
ATOM	147	CD	GLN	837	15.041	55.948	0.852	1.00100.00	6
ATOM	148	OE1	GLN	837	15.798	56.108	-0.108	1.00100.00	8
ATOM	149	NE2	GLN	837	14.796	56.912	1.739	1.00100.00	7
ATOM	150	C	GLN	837	13.327	51.889	1.138	1.00100.00	6
ATOM	151	O	GLN	837	12.525	52.818	1.236	1.00100.00	8
ATOM	152	N	VAL	838	12.993	50.652	0.789	1.00 49.78	7
ATOM	153	CA	VAL	838	11.645	50.199	0.469	1.00 49.78	6
ATOM	154	CB	VAL	838	11.565	48.683	0.604	1.00 54.51	6
ATOM	155	CG1	VAL	838	11.159	48.064	-0.703	1.00 54.51	6
ATOM	156	CG2	VAL	838	12.902	48.146	1.071	1.00 54.51	6
ATOM	157	C	VAL	838	10.515	50.785	1.303	1.00 49.78	6
ATOM	158	O	VAL	838	10.694	51.096	2.481	1.00 49.78	8
ATOM	159	N	LEU	839	9.344	50.916	0.684	1.00 44.19	7
ATOM	160	CA	LEU	839	8.171	51.461	1.369	1.00 44.19	6
ATOM	161	CB	LEU	839	7.935	52.921	0.962	1.00 90.21	6

FIG. 3C

ATOM	162	CG	LEU	839	9.039	53.975	1.060	1.00	84.90	6
ATOM	163	CD1	LEU	839	10.061	53.788	-0.028	1.00	84.90	6
ATOM	164	CD2	LEU	839	8.417	55.343	0.924	1.00	84.90	6
ATOM	165	C	LEU	839	6.900	50.671	1.061	1.00	44.19	6
ATOM	166	O	LEU	839	6.814	50.010	0.033	1.00	44.19	8
ATOM	167	N	LYS	840	5.920	50.740	1.959	1.00	64.49	7
ATOM	168	CA	LYS	840	4.642	50.068	1.744	1.00	64.49	6
ATOM	169	CB	LYS	840	3.953	49.727	3.066	1.00	84.80	6
ATOM	170	CG	LYS	840	2.531	49.222	2.900	1.00	81.21	6
ATOM	171	CD	LYS	840	2.073	48.506	4.142	1.00	81.21	6
ATOM	172	CE	LYS	840	0.582	48.660	4.331	1.00	81.21	6
ATOM	173	NZ	LYS	840	-0.153	48.279	3.096	1.00	81.21	7
ATOM	174	C	LYS	840	3.798	51.053	0.951	1.00	64.49	6
ATOM	175	O	LYS	840	3.854	52.260	1.176	1.00	64.49	8
ATOM	176	N	ALA	841	3.021	50.538	0.016	1.00	53.58	7
ATOM	177	CA	ALA	841	2.219	51.409	-0.814	1.00	53.58	6
ATOM	178	CB	ALA	841	3.082	51.913	-1.961	1.00	25.05	6
ATOM	179	C	ALA	841	1.003	50.670	-1.353	1.00	53.58	6
ATOM	180	O	ALA	841	1.144	49.616	-1.966	1.00	53.58	8
ATOM	181	N	ARG	842	-0.189	51.212	-1.135	1.00	86.10	7
ATOM	182	CA	ARG	842	-1.385	50.551	-1.637	1.00	86.10	6
ATOM	183	CB	ARG	842	-2.630	51.062	-0.905	1.00	40.66	6
ATOM	184	C	ARG	842	-1.514	50.804	-3.137	1.00	86.10	6
ATOM	185	O	ARG	842	-2.277	51.662	-3.572	1.00	86.10	8
ATOM	186	N	ILE	843	-0.763	50.040	-3.918	1.00	81.66	7
ATOM	187	CA	ILE	843	-0.773	50.176	-5.372	1.00	81.66	6
ATOM	188	CB	ILE	843	0.612	49.831	-5.984	1.00	100.00	6
ATOM	189	CG2	ILE	843	0.443	49.166	-7.362	1.00	100.00	6
ATOM	190	CG1	ILE	843	1.469	51.092	-6.056	1.00	100.00	6
ATOM	191	CD1	ILE	843	1.562	51.810	-4.732	1.00	100.00	6
ATOM	192	C	ILE	843	-1.796	49.337	-6.116	1.00	81.66	6
ATOM	193	O	ILE	843	-1.940	48.137	-5.884	1.00	81.66	8
ATOM	194	N	LYS	844	-2.482	49.988	-7.041	1.00	89.28	7
ATOM	195	CA	LYS	844	-3.449	49.324	-7.893	1.00	89.28	6
ATOM	196	CB	LYS	844	-4.657	50.218	-8.114	1.00	80.56	6
ATOM	197	C	LYS	844	-2.695	49.129	-9.205	1.00	89.28	6
ATOM	198	O	LYS	844	-1.818	49.928	-9.538	1.00	89.28	8
ATOM	199	N	LYS	845	-3.022	48.079	-9.944	1.00	100.00	7
ATOM	200	CA	LYS	845	-2.339	47.828	-11.208	1.00	100.00	6
ATOM	201	CB	LYS	845	-1.937	46.355	-11.305	1.00	100.00	6
ATOM	202	C	LYS	845	-3.232	48.203	-12.376	1.00	100.00	6
ATOM	203	O	LYS	845	-3.957	49.206	-12.324	1.00	100.00	8
ATOM	204	N	ASP	846	-2.834	47.343	-13.559	1.00	100.00	7
ATOM	205	CA	ASP	846	-3.726	47.631	-14.691	1.00	100.00	6
ATOM	206	CB	ASP	846	-3.314	46.796	-15.906	1.00	100.00	6
ATOM	207	CG	ASP	846	-3.993	47.249	-17.201	1.00	100.00	6
ATOM	208	OD1	ASP	846	-4.145	48.507	-17.444	1.00	100.00	8
ATOM	209	OD2	ASP	846	-4.414	46.373	-18.049	1.00	100.00	8
ATOM	210	C	ASP	846	-5.170	47.288	-14.320	1.00	100.00	6
ATOM	211	O	ASP	846	-5.989	46.948	-15.186	1.00	100.00	8
ATOM	212	N	GLY	847	-5.433	47.392	-13.030	1.00	100.00	7
ATOM	213	CA	GLY	847	-6.758	47.112	-12.459	1.00	100.00	6
ATOM	214	C	GLY	847	-6.612	46.491	-11.067	1.00	100.00	6
ATOM	215	O	GLY	847	-5.794	45.583	-10.856	1.00	100.00	8
ATOM	216	N	LEU	848	-7.419	47.011	-10.161	1.00	86.45	7
ATOM	217	CA	LEU	848	-7.450	46.563	-8.761	1.00	86.45	6
ATOM	218	CB	LEU	848	-7.206	45.055	-8.687	1.00	99.14	6

FIG. 3D

ATOM	219	CG	LEU	848	-6.201	44.560	-9.729	1.00	92.74	6
ATOM	220	CD1	LEU	848	-5.757	43.115	-9.491	1.00	92.74	6
ATOM	221	CD2	LEU	848	-6.753	44.595	-11.155	1.00	92.74	6
ATOM	222	C	LEU	848	-6.366	47.280	-7.954	1.00	86.45	6
ATOM	223	O	LEU	848	-5.717	48.215	-8.445	1.00	86.45	8
ATOM	224	N	ARG	849	-6.211	46.809	-6.730	1.00	99.60	7
ATOM	225	CA	ARG	849	-5.226	47.347	-5.780	1.00	99.60	6
ATOM	226	CB	ARG	849	-5.877	48.415	-4.899	1.00	100.00	6
ATOM	227	CG	ARG	849	-6.736	49.403	-5.692	1.00	99.93	6
ATOM	228	CD	ARG	849	-8.059	49.736	-4.998	1.00	99.93	6
ATOM	229	NE	ARG	849	-7.887	50.134	-3.594	1.00	99.93	7
ATOM	230	CZ	ARG	849	-8.903	50.347	-2.746	1.00	99.93	6
ATOM	231	NH1	ARG	849	-10.175	50.205	-3.143	1.00	99.93	7
ATOM	232	NH2	ARG	849	-8.747	50.710	-1.465	1.00	99.93	7
ATOM	233	C	ARG	849	-4.694	46.224	-4.887	1.00	99.60	6
ATOM	234	O	ARG	849	-5.398	45.242	-4.608	1.00	99.60	8
ATOM	235	N	MET	850	-3.457	46.411	-4.467	1.00	80.73	7
ATOM	236	CA	MET	850	-2.754	45.456	-3.599	1.00	80.73	6
ATOM	237	CB	MET	850	-1.967	44.457	-4.450	1.00	100.00	6
ATOM	238	CG	MET	850	-2.734	43.994	-5.690	1.00	68.64	6
ATOM	239	SD	MET	850	-1.849	44.290	-7.206	1.00	68.64	16
ATOM	240	CE	MET	850	-0.189	43.661	-7.074	1.00	68.64	6
ATOM	241	C	MET	850	-1.782	46.199	-2.681	1.00	80.73	6
ATOM	242	O	MET	850	-1.937	47.403	-2.426	1.00	80.73	8
ATOM	243	N	ASP	851	-1.168	45.352	-2.147	1.00	74.44	7
ATOM	244	CA	ASP	851	-0.137	45.775	-1.223	1.00	74.44	6
ATOM	245	CB	ASP	851	-0.163	44.913	0.034	1.00	100.00	6
ATOM	246	CG	ASP	851	-0.724	45.642	1.229	1.00	100.00	6
ATOM	247	OD1	ASP	851	-1.307	46.731	1.026	1.00	100.00	8
ATOM	248	OD2	ASP	851	-0.588	45.124	2.360	1.00	100.00	8
ATOM	249	C	ASP	851	1.159	45.518	-1.967	1.00	74.44	6
ATOM	250	O	ASP	851	1.583	44.367	-2.118	1.00	74.44	8
ATOM	251	N	ALA	852	1.775	46.581	-2.456	1.00	26.66	7
ATOM	252	CA	ALA	852	3.023	46.431	-3.173	1.00	26.66	6
ATOM	253	CB	ALA	852	2.984	47.212	-4.475	1.00	11.17	6
ATOM	254	C	ALA	852	4.155	46.921	-2.313	1.00	26.66	6
ATOM	255	O	ALA	852	3.957	47.275	-1.154	1.00	26.66	8
ATOM	256	N	ALA	853	5.346	46.931	-2.890	1.00	89.52	7
ATOM	257	CA	ALA	853	6.532	47.410	-2.204	1.00	89.52	6
ATOM	258	CB	ALA	853	7.355	46.243	-1.675	1.00	23.28	6
ATOM	259	C	ALA	853	7.324	48.210	-3.229	1.00	89.52	6
ATOM	260	O	ALA	853	7.765	47.668	-4.240	1.00	89.52	8
ATOM	261	N	ILE	854	7.417	49.467	-3.319	1.00	41.73	7
ATOM	262	CA	ILE	854	8.279	50.444	-3.999	1.00	41.73	6
ATOM	263	CB	ILE	854	7.851	51.866	-3.630	1.00	71.42	6
ATOM	264	CG2	ILE	854	8.539	52.937	-4.479	1.00	83.27	6
ATOM	265	CG1	ILE	854	6.349	52.102	-3.802	1.00	83.27	6
ATOM	266	CD1	ILE	854	5.768	51.388	-5.024	1.00	83.27	6
ATOM	267	C	ILE	854	9.736	50.239	-3.577	1.00	41.73	6
ATOM	268	O	ILE	854	10.035	50.042	-2.390	1.00	41.73	8
ATOM	269	N	LYS	855	10.597	50.294	-4.576	1.00	62.34	7
ATOM	270	CA	LYS	855	12.045	50.123	-4.395	1.00	62.34	6
ATOM	271	CB	LYS	855	12.496	48.792	-5.001	1.00	99.81	6
ATOM	272	CG	LYS	855	13.652	48.147	-4.235	1.00	99.81	6
ATOM	273	CD	LYS	855	13.741	46.635	-4.449	1.00	99.81	6
ATOM	274	CE	LYS	855	13.407	46.212	-5.881	1.00	99.81	6
ATOM	275	NZ	LYS	855	14.507	46.460	-6.824	1.00	99.81	7

FIG. 3E

ATOM	276	C	LYS	855	12.797	51.263	-5.085	1.00 62.34	6
ATOM	277	O	LYS	855	12.216	52.028	-5.869	1.00 62.34	8
ATOM	278	N	ARG	856	14.076	51.334	-4.765	1.00100.00	7
ATOM	279	CA	ARG	856	14.982	52.353	-5.313	1.00100.00	6
ATOM	280	CB	ARG	856	14.324	53.733	-5.241	1.00 95.22	6
ATOM	281	CG	ARG	856	15.161	54.829	-5.903	1.00 95.22	6
ATOM	282	CD	ARG	856	14.465	56.192	-5.906	1.00 95.22	6
ATOM	283	NE	ARG	856	15.316	57.271	-6.428	1.00 95.22	7
ATOM	284	CZ	ARG	856	14.938	58.554	-6.503	1.00 95.22	6
ATOM	285	NH1	ARG	856	13.723	58.940	-6.093	1.00 95.22	7
ATOM	286	NH2	ARG	856	15.715	59.537	-6.979	1.00 95.22	7
ATOM	287	C	ARG	856	16.284	52.382	-4.510	1.00100.00	6
ATOM	288	O	ARG	856	16.269	52.404	-3.270	1.00100.00	8
ATOM	289	N	MET	857	17.443	52.378	-5.338	1.00100.00	7
ATOM	290	CA	MET	857	18.288	53.750	-3.743	1.00100.00	6
ATOM	291	CB	MET	857	18.449	53.097	-2.384	1.00100.00	6
ATOM	292	CG	MET	857	17.994	54.017	-1.306	1.00100.00	6
ATOM	293	SD	MET	857	18.352	53.350	0.258	1.00100.00	16
ATOM	294	CE	MET	857	20.116	53.447	0.204	1.00100.00	6
ATOM	295	C	MET	857	19.646	53.843	-4.450	1.00100.00	6
ATOM	296	O	MET	857	20.497	52.937	-4.253	1.00100.00	8
ATOM	297	OXT	MET	857	19.839	54.838	-5.196	1.00 82.10	8
TER									
ATOM	298	CB	ASP	864	22.499	59.975	-11.088	1.00 55.87	6
ATOM	299	C	ASP	864	23.323	58.318	-12.792	1.00100.00	6
ATOM	300	O	ASP	864	22.981	58.052	-13.940	1.00100.00	8
ATOM	301	N	ASP	864	22.263	57.542	-10.688	1.00100.00	7
ATOM	302	CA	ASP	864	22.263	58.615	-11.734	1.00100.00	6
ATOM	303	N	ASP	865	24.599	58.333	-12.412	1.00100.00	7
ATOM	304	CA	ASP	865	25.670	57.988	-13.347	1.00100.00	6
ATOM	305	CB	ASP	865	26.925	58.842	-13.098	1.00 87.31	6
ATOM	306	C	ASP	865	25.951	56.494	-13.073	1.00100.00	6
ATOM	307	O	ASP	865	26.537	55.781	-13.902	1.00100.00	8
ATOM	308	N	HIS	866	25.485	56.080	-11.889	1.00 99.63	7
ATOM	309	CA	HIS	866	25.554	54.713	-11.357	1.00 99.63	6
ATOM	310	CB	HIS	866	25.728	54.726	-9.827	1.00100.00	6
ATOM	311	CG	HIS	866	24.600	55.378	-9.079	1.00100.00	6
ATOM	312	CD2	HIS	866	23.472	54.858	-8.543	1.00100.00	6
ATOM	313	ND1	HIS	866	24.593	56.720	-8.769	1.00100.00	7
ATOM	314	CE1	HIS	866	23.509	57.002	-8.065	1.00100.00	6
ATOM	315	NE2	HIS	866	22.811	55.888	-7.915	1.00100.00	7
ATOM	316	C	HIS	866	24.196	54.120	-11.715	1.00 99.63	6
ATOM	317	O	HIS	866	23.599	53.339	-10.964	1.00 99.63	8
ATOM	318	N	ARG	867	23.732	54.498	-12.904	1.00100.00	7
ATOM	319	CA	ARG	867	22.419	54.106	-13.405	1.00100.00	6
ATOM	320	CB	ARG	867	21.700	55.371	-13.954	1.00100.00	6
ATOM	321	CG	ARG	867	21.971	55.721	-15.445	1.00100.00	6
ATOM	322	CD	ARG	867	23.460	55.680	-15.790	1.00100.00	6
ATOM	323	NE	ARG	867	23.698	55.859	-17.219	1.00100.00	7
ATOM	324	CZ	ARG	867	24.794	55.439	-17.837	1.00100.00	6
ATOM	325	NH1	ARG	867	25.733	54.810	-17.137	1.00100.00	7
ATOM	326	NH2	ARG	867	24.940	55.628	-19.145	1.00100.00	7
ATOM	327	C	ARG	867	22.524	53.015	-14.480	1.00100.00	6
ATOM	328	O	ARG	867	21.980	53.140	-15.575	1.00100.00	8
ATOM	329	N	ASP	868	23.225	51.934	-14.164	1.00100.00	7
ATOM	330	CA	ASP	868	23.393	50.867	-15.146	1.00100.00	6
ATOM	331	CB	ASP	868	24.591	49.998	-14.773	1.00100.00	6

FIG. 3F

ATOM	332	CG	ASP	868	24.412	49.314	-13.435	1.00100.00	6
ATOM	333	OD1	ASP	868	24.613	49.980	-12.391	1.00100.00	8
ATOM	334	OD2	ASP	868	24.027	48.130	-13.442	1.00100.00	8
ATOM	335	C	ASP	868	22.154	49.960	-15.282	1.00100.00	6
ATOM	336	O	ASP	868	22.293	48.750	-15.504	1.00100.00	8
ATOM	337	N	PHE	869	20.955	50.538	-15.156	1.00100.00	7
ATOM	338	CA	PHE	869	19.717	49.746	-15.259	1.00100.00	6
ATOM	339	CB	PHE	869	18.424	50.554	-15.017	1.00 99.62	6
ATOM	340	CG	PHE	869	18.595	52.044	-14.986	1.00 99.62	6
ATOM	341	CD1	PHE	869	18.716	52.692	-13.761	1.00 99.62	6
ATOM	342	CD2	PHE	869	18.498	52.813	-16.148	1.00 99.62	6
ATOM	343	CE1	PHE	869	18.734	54.068	-13.681	1.00 99.62	6
ATOM	344	CE2	PHE	869	18.515	54.204	-16.077	1.00 99.62	6
ATOM	345	CZ	PHE	869	18.630	54.834	-14.843	1.00 99.62	6
ATOM	346	C	PHE	869	19.576	49.080	-16.612	1.00100.00	6
ATOM	347	O	PHE	869	20.380	49.305	-17.508	1.00100.00	8
ATOM	348	N	ALA	870	18.524	48.278	-16.746	1.00100.00	7
ATOM	349	CA	ALA	870	18.206	47.512	-17.951	1.00100.00	6
ATOM	350	CB	ALA	870	19.005	48.006	-19.156	1.00 97.10	6
ATOM	351	C	ALA	870	18.532	46.061	-17.670	1.00100.00	6
ATOM	352	O	ALA	870	17.644	45.222	-17.671	1.00100.00	8
ATOM	353	N	GLY	871	19.810	45.775	-17.434	1.00100.00	7
ATOM	354	CA	GLY	871	20.221	44.419	-17.133	1.00100.00	6
ATOM	355	C	GLY	871	19.602	44.044	-15.804	1.00100.00	6
ATOM	356	O	GLY	871	19.400	42.871	-15.506	1.00100.00	8
ATOM	357	N	GLU	872	19.305	45.055	-14.996	1.00 99.97	7
ATOM	358	CA	GLU	872	18.669	44.813	-13.718	1.00 99.97	6
ATOM	359	CB	GLU	872	18.811	46.023	-12.787	1.00100.00	6
ATOM	360	CG	GLU	872	17.496	46.495	-12.182	1.00100.00	6
ATOM	361	CD	GLU	872	17.571	46.692	-10.675	1.00100.00	6
ATOM	362	OE1	GLU	872	18.323	47.585	-10.230	1.00100.00	8
ATOM	363	OE2	GLU	872	16.882	45.946	-9.940	1.00100.00	8
ATOM	364	C	GLU	872	17.200	44.565	-14.033	1.00 99.97	6
ATOM	365	O	GLU	872	16.575	43.673	-13.465	1.00 99.97	8
ATOM	366	N	LEU	873	16.659	45.350	-14.961	1.00 63.02	7
ATOM	367	CA	LEU	873	15.255	45.213	-15.327	1.00 63.02	6
ATOM	368	CB	LEU	873	14.756	46.482	-15.955	1.00 69.97	6
ATOM	369	C	LEU	873	14.977	44.032	-16.243	1.00 63.02	6
ATOM	370	O	LEU	873	13.990	43.323	-16.052	1.00 63.02	8
ATOM	371	N	GLU	874	15.847	43.819	-17.227	1.00100.00	7
ATOM	372	CA	GLU	874	15.687	42.716	-18.164	1.00100.00	6
ATOM	373	CB	GLU	874	16.645	42.862	-19.331	1.00 19.50	6
ATOM	374	C	GLU	874	15.923	41.394	-17.454	1.00100.00	6
ATOM	375	O	GLU	874	15.103	40.482	-17.547	1.00100.00	8
ATOM	376	N	VAL	875	17.040	41.298	-16.737	1.00 69.27	7
ATOM	377	CA	VAL	875	17.383	40.082	-16.002	1.00 69.27	6
ATOM	378	CB	VAL	875	18.763	40.218	-15.359	1.00 39.27	6
ATOM	379	C	VAL	875	16.344	39.755	-14.934	1.00 69.27	6
ATOM	380	O	VAL	875	16.338	38.651	-14.399	1.00 69.27	8
ATOM	381	N	LEU	876	15.493	40.728	-14.613	1.00 78.00	7
ATOM	382	CA	LEU	876	14.438	40.543	-13.616	1.00 78.00	6
ATOM	383	CB	LEU	876	14.169	41.853	-12.843	1.00 53.20	6
ATOM	384	CG	LEU	876	14.939	42.141	-11.537	1.00 29.26	6
ATOM	385	CD1	LEU	876	14.466	43.420	-10.852	1.00 29.26	6
ATOM	386	CD2	LEU	876	14.715	40.969	-10.608	1.00 29.26	6
ATOM	387	C	LEU	876	13.147	40.076	-14.290	1.00 78.00	6
ATOM	388	O	LEU	876	12.410	39.262	-13.737	1.00 78.00	8

FIG. 3G

ATOM	389	N	CYS	877	12.870	40.591	-15.486	1.00	60.18	7
ATOM	390	CA	CYS	877	11.652	40.208	-16.191	1.00	60.18	6
ATOM	391	CB	CYS	877	11.199	41.317	-17.164	1.00	100.00	6
ATOM	392	SG	CYS	877	12.370	41.807	-18.447	1.00	100.00	16
ATOM	393	C	CYS	877	11.857	38.886	-16.916	1.00	60.18	6
ATOM	394	O	CYS	877	11.194	38.591	-17.909	1.00	60.18	8
ATOM	395	N	LYS	878	12.788	38.094	-16.398	1.00	65.17	7
ATOM	396	CA	LYS	878	13.088	36.788	-16.964	1.00	65.17	6
ATOM	397	CB	LYS	878	14.593	36.609	-17.078	1.00	89.20	6
ATOM	398	CG	LYS	878	15.190	37.551	-18.092	1.00	52.09	6
ATOM	399	CD	LYS	878	16.693	37.453	-18.128	1.00	52.09	6
ATOM	400	CE	LYS	878	17.289	38.360	-19.216	1.00	52.09	6
ATOM	401	NZ	LYS	878	16.965	37.922	-20.614	1.00	52.09	7
ATOM	402	C	LYS	878	12.473	35.703	-16.091	1.00	65.17	6
ATOM	403	O	LYS	878	12.100	34.632	-16.572	1.00	65.17	8
ATOM	404	N	LEU	879	12.365	35.982	-14.801	1.00	100.00	7
ATOM	405	CA	LEU	879	11.752	35.044	-13.879	1.00	100.00	6
ATOM	406	CB	LEU	879	12.480	35.052	-12.526	1.00	45.22	6
ATOM	407	CG	LEU	879	12.801	36.419	-11.904	1.00	46.30	6
ATOM	408	CD1	LEU	879	13.226	36.250	-10.462	1.00	46.30	6
ATOM	409	CD2	LEU	879	13.892	37.109	-12.704	1.00	46.30	6
ATOM	410	C	LEU	879	10.301	35.492	-13.717	1.00	100.00	6
ATOM	411	O	LEU	879	10.019	36.656	-13.405	1.00	100.00	8
ATOM	412	N	GLY	880	9.381	34.572	-13.972	1.00	96.05	7
ATOM	413	CA	GLY	880	7.980	34.903	-13.848	1.00	96.05	6
ATOM	414	C	GLY	880	7.540	34.784	-12.409	1.00	96.05	6
ATOM	415	O	GLY	880	8.358	34.825	-11.483	1.00	96.05	8
ATOM	416	N	HIS	881	6.236	34.641	-12.216	1.00	70.51	7
ATOM	417	CA	HIS	881	5.693	34.496	-10.876	1.00	70.51	6
ATOM	418	CB	HIS	881	4.178	34.726	-10.843	1.00	99.80	6
ATOM	419	CG	HIS	881	3.498	34.160	-9.629	1.00	99.80	6
ATOM	420	CD2	HIS	881	3.000	32.924	-9.383	1.00	99.80	6
ATOM	421	ND1	HIS	881	3.264	34.897	-8.484	1.00	99.80	7
ATOM	422	CE1	HIS	881	2.648	34.142	-7.592	1.00	99.80	6
ATOM	423	NE2	HIS	881	2.477	32.939	-8.110	1.00	99.80	7
ATOM	424	C	HIS	881	5.952	33.094	-10.384	1.00	70.51	6
ATOM	425	O	HIS	881	5.908	32.134	-11.147	1.00	70.51	8
ATOM	426	N	HIS	882	6.231	32.982	-9.104	1.00	45.83	7
ATOM	427	CA	HIS	882	6.404	31.672	-8.546	1.00	45.83	6
ATOM	428	CB	HIS	882	7.866	31.289	-8.449	1.00	14.81	6
ATOM	429	CG	HIS	882	8.076	29.813	-8.295	1.00	29.81	6
ATOM	430	CD2	HIS	882	7.783	28.782	-9.126	1.00	29.81	6
ATOM	431	ND1	HIS	882	8.608	29.244	-7.167	1.00	29.81	7
ATOM	432	CE1	HIS	882	8.638	27.932	-7.299	1.00	29.81	6
ATOM	433	NE2	HIS	882	8.142	27.626	-8.484	1.00	29.81	7
ATOM	434	C	HIS	882	5.773	31.719	-7.182	1.00	45.83	6
ATOM	435	O	HIS	882	5.987	32.655	-6.411	1.00	45.83	8
ATOM	436	N	PRO	883	4.959	30.711	-6.873	1.00	37.21	7
ATOM	437	CD	PRO	883	4.747	29.405	-7.508	1.00	52.55	6
ATOM	438	CA	PRO	883	4.353	30.762	-5.556	1.00	37.21	6
ATOM	439	CB	PRO	883	3.821	29.336	-5.373	1.00	47.02	6
ATOM	440	CG	PRO	883	4.591	28.493	-6.316	1.00	52.55	6
ATOM	441	C	PRO	883	5.359	31.209	-4.487	1.00	37.21	6
ATOM	442	O	PRO	883	4.990	31.958	-3.579	1.00	37.21	8
ATOM	443	N	ASN	884	6.628	30.800	-4.601	1.00	24.86	7
ATOM	444	CA	ASN	884	7.619	31.198	-3.582	1.00	24.86	6
ATOM	445	CB	ASN	884	8.077	29.996	-2.714	1.00	18.47	6

FIG. 3H

ATOM	446	CG	ASN	884	7.553	28.671	-3.203	1.00 33.47	6
ATOM	447	OD1	ASN	884	7.951	28.205	-4.243	1.00 33.47	8
ATOM	448	ND2	ASN	884	6.674	28.052	-2.443	1.00 33.47	7
ATOM	449	C	ASN	884	8.860	31.986	-4.022	1.00 24.86	6
ATOM	450	O	ASN	884	9.996	31.540	-3.862	1.00 24.86	8
ATOM	451	N	ILE	885	8.603	33.191	-4.518	1.00 46.00	7
ATOM	452	CA	ILE	885	9.616	34.125	-4.986	1.00 46.00	6
ATOM	453	CB	ILE	885	10.063	33.811	-6.435	1.00 25.68	6
ATOM	454	CG2	ILE	885	10.616	35.056	-7.119	1.00 21.87	6
ATOM	455	CG1	ILE	885	11.101	32.696	-6.451	1.00 21.87	6
ATOM	456	CD1	ILE	885	11.855	32.614	-7.727	1.00 21.87	6
ATOM	457	C	ILE	885	8.924	35.476	-5.013	1.00 46.00	6
ATOM	458	O	ILE	885	7.845	35.596	-5.601	1.00 46.00	8
ATOM	459	N	ILE	886	9.501	36.488	-4.373	1.00 36.62	7
ATOM	460	CA	ILE	886	8.857	37.785	-4.434	1.00 36.62	6
ATOM	461	CB	ILE	886	9.462	38.768	-3.414	1.00 17.99	6
ATOM	462	CG2	ILE	886	9.259	40.221	-3.846	1.00 27.09	6
ATOM	463	CG1	ILE	886	8.764	38.531	-2.075	1.00 27.09	6
ATOM	464	CD1	ILE	886	9.230	39.402	-1.000	1.00 27.09	6
ATOM	465	C	ILE	886	8.969	38.250	-5.881	1.00 36.62	6
ATOM	466	O	ILE	886	10.040	38.615	-6.363	1.00 36.62	8
ATOM	467	N	ASN	887	7.832	38.163	-6.566	1.00 39.60	7
ATOM	468	CA	ASN	887	7.716	38.506	-7.975	1.00 39.60	6
ATOM	469	CB	ASN	887	6.531	37.759	-8.603	1.00 82.94	6
ATOM	470	CG	ASN	887	6.602	36.250	-8.406	1.00 82.94	6
ATOM	471	OD1	ASN	887	7.490	35.584	-8.932	1.00 82.94	8
ATOM	472	ND2	ASN	887	5.665	35.710	-7.637	1.00 82.94	7
ATOM	473	C	ASN	887	7.535	39.990	-8.222	1.00 39.60	6
ATOM	474	O	ASN	887	6.893	40.687	-7.432	1.00 39.60	8
ATOM	475	N	LEU	888	8.125	40.438	-9.332	1.00 73.28	7
ATOM	476	CA	LEU	888	8.067	41.822	-9.789	1.00 73.28	6
ATOM	477	CB	LEU	888	9.044	42.055	-10.953	1.00 34.36	6
ATOM	478	CG	LEU	888	9.064	43.390	-11.721	1.00 18.51	6
ATOM	479	CD1	LEU	888	9.760	44.444	-10.873	1.00 18.51	6
ATOM	480	CD2	LEU	888	9.809	43.220	-13.035	1.00 18.51	6
ATOM	481	C	LEU	888	6.651	42.083	-10.274	1.00 73.28	6
ATOM	482	O	LEU	888	6.083	41.282	-11.022	1.00 73.28	8
ATOM	483	N	LEU	889	6.091	43.210	-9.853	1.00 99.59	7
ATOM	484	CA	LEU	889	4.731	43.573	-10.235	1.00 99.59	6
ATOM	485	CB	LEU	889	3.936	43.972	-8.975	1.00 97.88	6
ATOM	486	CG	LEU	889	3.874	42.924	-7.838	1.00 59.80	6
ATOM	487	CD1	LEU	889	2.923	43.357	-6.733	1.00 59.80	6
ATOM	488	CD2	LEU	889	3.419	41.589	-8.413	1.00 59.80	6
ATOM	489	C	LEU	889	4.676	44.676	-11.304	1.00 99.59	6
ATOM	490	O	LEU	889	3.805	44.645	-12.167	1.00 99.59	8
ATOM	491	N	GLY	890	5.599	45.636	-11.266	1.00 54.35	7
ATOM	492	CA	GLY	890	5.597	46.699	-12.264	1.00 54.35	6
ATOM	493	C	GLY	890	6.668	47.737	-11.986	1.00 54.35	6
ATOM	494	O	GLY	890	7.617	47.466	-11.259	1.00 54.35	8
ATOM	495	N	ALA	891	6.534	48.926	-12.560	1.00 66.65	7
ATOM	496	CA	ALA	891	7.515	49.985	-12.328	1.00 66.65	6
ATOM	497	CB	ALA	891	8.872	49.590	-12.911	1.00 68.11	6
ATOM	498	C	ALA	891	7.055	51.299	-12.937	1.00 66.65	6
ATOM	499	O	ALA	891	6.176	51.318	-13.789	1.00 66.65	8
ATOM	500	N	CYS	892	7.656	52.393	-12.485	1.00 99.57	7
ATOM	501	CA	CYS	892	7.322	53.720	-12.984	1.00 99.57	6
ATOM	502	CB	CYS	892	6.872	54.619	-11.833	1.00 98.88	6

FIG. 3I

ATOM	503	SG	CYS	892	5.614	55.803	-12.345	1.00 92.24	16
ATOM	504	C	CYS	892	8.579	54.284	-13.611	1.00 99.57	6
ATOM	505	O	CYS	892	9.610	53.625	-13.607	1.00 99.57	8
ATOM	506	N	GLU	893	8.503	55.485	-14.165	1.00 99.69	7
ATOM	507	CA	GLU	893	9.676	56.130	-14.759	1.00 99.69	6
ATOM	508	CB	GLU	893	9.687	55.991	-16.289	1.00100.00	6
ATOM	509	CG	GLU	893	10.439	54.776	-16.825	1.00100.00	6
ATOM	510	CD	GLU	893	10.793	54.883	-18.308	1.00100.00	6
ATOM	511	OE1	GLU	893	11.715	55.657	-18.646	1.00100.00	8
ATOM	512	OE2	GLU	893	10.123	54.219	-19.128	1.00100.00	8
ATOM	513	C	GLU	893	9.616	57.594	-14.387	1.00 99.69	6
ATOM	514	O	GLU	893	9.817	58.469	-15.215	1.00 99.69	8
ATOM	515	N	HIS	894	9.516	57.779	-12.908	1.00 96.96	7
ATOM	516	CA	HIS	894	9.344	59.158	-12.428	1.00 96.96	6
ATOM	517	CB	HIS	894	8.697	59.154	-11.042	1.00100.00	6
ATOM	518	CG	HIS	894	8.186	60.532	-10.618	1.00100.00	6
ATOM	519	CD2	HIS	894	7.291	61.381	-11.187	1.00100.00	6
ATOM	520	ND1	HIS	894	8.631	61.157	-9.457	1.00100.00	7
ATOM	521	CE1	HIS	894	8.019	62.323	-9.357	1.00100.00	6
ATOM	522	NE2	HIS	894	7.216	62.472	-10.381	1.00100.00	7
ATOM	523	C	HIS	894	10.703	59.854	-12.336	1.00 96.96	6
ATOM	524	O	HIS	894	11.756	59.200	-12.319	1.00 96.96	8
ATOM	525	N	ARG	895	10.631	61.171	-12.278	1.00100.00	7
ATOM	526	CA	ARG	895	11.818	62.033	-12.182	1.00100.00	6
ATOM	527	CB	ARG	895	11.408	63.440	-11.741	1.00100.00	6
ATOM	528	CG	ARG	895	10.703	64.230	-12.846	1.00100.00	6
ATOM	529	CD	ARG	895	10.357	65.661	-12.430	1.00100.00	6
ATOM	530	NE	ARG	895	10.896	66.673	-13.350	1.00100.00	7
ATOM	531	CZ	ARG	895	10.138	67.483	-14.101	1.00100.00	6
ATOM	532	NH1	ARG	895	8.801	67.415	-14.056	1.00100.00	7
ATOM	533	NH2	ARG	895	10.630	68.406	-14.939	1.00100.00	7
ATOM	534	C	ARG	895	12.796	61.452	-11.159	1.00100.00	6
ATOM	535	O	ARG	895	12.399	60.726	-10.236	1.00100.00	8
ATOM	536	N	GLY	896	14.055	61.795	-11.359	1.00100.00	7
ATOM	537	CA	GLY	896	15.150	61.337	-10.493	1.00100.00	6
ATOM	538	C	GLY	896	14.949	59.861	-10.145	1.00100.00	6
ATOM	539	O	GLY	896	14.575	59.517	-9.013	1.00100.00	8
ATOM	540	N	TYR	897	15.205	59.037	-11.143	1.00100.00	7
ATOM	541	CA	TYR	897	15.068	57.578	-11.033	1.00100.00	6
ATOM	542	CB	TYR	897	15.624	57.096	-9.692	1.00100.00	6
ATOM	543	CG	TYR	897	15.964	55.604	-9.688	1.00100.00	6
ATOM	544	CD1	TYR	897	17.195	55.165	-10.192	1.00100.00	6
ATOM	545	CE1	TYR	897	17.506	53.800	-10.190	1.00100.00	6
ATOM	546	CD2	TYR	897	15.045	54.676	-9.182	1.00100.00	6
ATOM	547	CE2	TYR	897	15.357	53.311	-9.179	1.00100.00	6
ATOM	548	CZ	TYR	897	16.587	52.873	-9.684	1.00100.00	6
ATOM	549	OH	TYR	897	16.890	51.547	-9.682	1.00100.00	8
ATOM	550	C	TYR	897	13.592	57.190	-11.131	1.00100.00	6
ATOM	551	O	TYR	897	12.714	58.051	-11.293	1.00100.00	8
ATOM	552	N	LEU	898	13.367	55.894	-11.027	1.00100.00	7
ATOM	553	CA	LEU	898	12.020	55.310	-11.093	1.00100.00	6
ATOM	554	CB	LEU	898	11.960	54.258	-12.202	1.00 41.85	6
ATOM	555	C	LEU	898	11.672	54.648	-9.759	1.00100.00	6
ATOM	556	O	LEU	898	12.234	54.992	-8.709	1.00100.00	8
ATOM	557	N	TYR	899	10.747	53.711	-9.850	1.00 72.77	7
ATOM	558	CA	TYR	899	10.267	52.951	-8.688	1.00 72.77	6
ATOM	559	CB	TYR	899	9.153	53.725	-7.982	1.00100.00	6

FIG. 3J

ATOM	560	CG	TYR	899	9.685	54.728	-6.958	1.00100.00	6
ATOM	561	CD1	TYR	899	9.394	56.090	-7.096	1.00100.00	6
ATOM	562	CE1	TYR	899	9.884	57.008	-6.159	1.00100.00	6
ATOM	563	CD2	TYR	899	10.465	54.283	-5.884	1.00100.00	6
ATOM	564	CE2	TYR	899	10.955	55.201	-4.948	1.00100.00	6
ATOM	565	CZ	TYR	899	10.664	56.564	-5.085	1.00100.00	6
ATOM	566	OH	TYR	899	11.140	57.456	-4.175	1.00100.00	8
ATOM	567	C	TYR	899	9.726	51.592	-9.136	1.00 72.77	6
ATOM	568	O	TYR	899	8.785	51.513	-9.940	1.00 72.77	8
ATOM	569	N	LEU	900	10.350	50.565	-8.591	1.00 78.27	7
ATOM	570	CA	LEU	900	9.996	49.168	-8.876	1.00 78.27	6
ATOM	571	CB	LEU	900	11.233	48.277	-8.738	1.00 79.18	6
ATOM	572	CG	LEU	900	11.566	47.512	-10.020	1.00 54.43	6
ATOM	573	CD1	LEU	900	11.602	48.408	-11.259	1.00 54.43	6
ATOM	574	CD2	LEU	900	12.931	46.823	-9.967	1.00 54.43	6
ATOM	575	C	LEU	900	8.927	48.689	-7.892	1.00 78.27	6
ATOM	576	O	LEU	900	9.079	48.823	-6.669	1.00 78.27	8
ATOM	577	N	ALA	901	7.874	48.141	-8.468	1.00 72.23	7
ATOM	578	CA	ALA	901	6.731	47.614	-7.708	1.00 72.23	6
ATOM	579	CB	ALA	901	5.424	47.944	-8.433	1.00 33.79	6
ATOM	580	C	ALA	901	6.851	46.095	-7.568	1.00 72.23	6
ATOM	581	O	ALA	901	7.121	45.383	-8.546	1.00 72.23	8
ATOM	582	N	ILE	902	6.929	45.582	-6.293	1.00 59.87	7
ATOM	583	CA	ILE	902	7.104	44.154	-6.059	1.00 59.87	6
ATOM	584	CB	ILE	902	8.550	43.900	-5.623	1.00 34.80	6
ATOM	585	CG2	ILE	902	9.522	44.289	-6.729	1.00 35.77	6
ATOM	586	CG1	ILE	902	8.846	44.755	-4.397	1.00 35.77	6
ATOM	587	CD1	ILE	902	10.311	45.018	-4.169	1.00 35.77	6
ATOM	588	C	ILE	902	6.165	43.633	-4.969	1.00 59.87	6
ATOM	589	O	ILE	902	5.750	44.390	-4.093	1.00 59.87	8
ATOM	590	N	GLU	903	5.835	42.344	-5.030	1.00 34.73	7
ATOM	591	CA	GLU	903	4.967	41.716	-4.036	1.00 34.73	6
ATOM	592	CB	GLU	903	5.047	40.197	-4.119	1.00 38.01	6
ATOM	593	CG	GLU	903	4.180	39.568	-5.170	1.00 49.25	6
ATOM	594	CD	GLU	903	4.216	38.043	-5.112	1.00 49.25	6
ATOM	595	OE1	GLU	903	4.310	37.497	-3.985	1.00 49.25	8
ATOM	596	OE2	GLU	903	4.141	37.403	-6.191	1.00 49.25	8
ATOM	597	C	GLU	903	5.343	42.124	-2.627	1.00 34.73	6
ATOM	598	O	GLU	903	6.514	42.378	-2.330	1.00 34.73	8
ATOM	599	N	TYR	904	4.328	42.169	-1.770	1.00 31.03	7
ATOM	600	CA	TYR	904	4.469	42.530	-0.370	1.00 31.03	6
ATOM	601	CB	TYR	904	3.411	43.577	-0.003	1.00 13.64	6
ATOM	602	CG	TYR	904	3.419	43.950	1.459	1.00 23.21	6
ATOM	603	CD1	TYR	904	4.598	44.344	2.086	1.00 23.21	6
ATOM	604	CE1	TYR	904	4.647	44.606	3.448	1.00 23.21	6
ATOM	605	CD2	TYR	904	2.276	43.840	2.236	1.00 23.21	6
ATOM	606	CE2	TYR	904	2.315	44.102	3.608	1.00 23.21	6
ATOM	607	CZ	TYR	904	3.509	44.477	4.204	1.00 23.21	6
ATOM	608	OH	TYR	904	3.575	44.663	5.569	1.00 23.21	8
ATOM	609	C	TYR	904	4.328	41.291	0.532	1.00 31.03	6
ATOM	610	O	TYR	904	3.388	40.494	0.393	1.00 31.03	8
ATOM	611	N	ALA	905	5.284	41.154	1.447	1.00 31.20	7
ATOM	612	CA	ALA	905	5.334	40.063	2.409	1.00 31.20	6
ATOM	613	CB	ALA	905	6.733	39.460	2.430	1.00 28.71	6
ATOM	614	C	ALA	905	4.990	40.633	3.781	1.00 31.20	6
ATOM	615	O	ALA	905	5.853	41.091	4.514	1.00 31.20	8
ATOM	616	N	PRO	906	3.716	40.600	4.151	1.00 17.48	7

FIG. 3K

ATOM	617	CD	PRO	906	2.597	40.048	3.370	1.00	32.19	6
ATOM	618	CA	PRO	906	3.241	41.121	5.427	1.00	17.48	6
ATOM	619	CB	PRO	906	1.728	40.964	5.314	1.00	32.19	6
ATOM	620	CG	PRO	906	1.580	39.762	4.442	1.00	32.19	6
ATOM	621	C	PRO	906	3.774	40.564	6.724	1.00	17.48	6
ATOM	622	O	PRO	906	3.408	41.072	7.788	1.00	17.48	8
ATOM	623	N	HIS	907	4.636	39.550	6.683	1.00	30.66	7
ATOM	624	CA	HIS	907	5.123	38.987	7.954	1.00	30.66	6
ATOM	625	CB	HIS	907	4.657	37.543	8.130	1.00	5.00	6
ATOM	626	CG	HIS	907	3.174	37.357	8.048	1.00	5.00	6
ATOM	627	CD2	HIS	907	2.219	37.353	9.011	1.00	5.00	6
ATOM	628	ND1	HIS	907	2.517	37.103	6.865	1.00	5.00	7
ATOM	629	CE1	HIS	907	1.224	36.945	7.097	1.00	5.00	6
ATOM	630	NE2	HIS	907	1.021	37.091	8.393	1.00	5.00	7
ATOM	631	C	HIS	907	6.622	39.004	8.229	1.00	30.66	6
ATOM	632	O	HIS	907	7.130	38.115	8.926	1.00	30.66	8
ATOM	633	N	GLY	908	7.326	40.009	7.718	1.00	38.98	7
ATOM	634	CA	GLY	908	8.756	40.081	7.947	1.00	38.98	6
ATOM	635	C	GLY	908	9.483	38.924	7.298	1.00	38.98	6
ATOM	636	O	GLY	908	8.935	38.235	6.436	1.00	38.98	8
ATOM	637	N	ASN	909	10.719	38.698	7.718	1.00	31.42	7
ATOM	638	CA	ASN	909	11.517	37.620	7.140	1.00	31.42	6
ATOM	639	CB	ASN	909	12.963	38.068	6.941	1.00	41.70	6
ATOM	640	CG	ASN	909	13.566	38.630	8.197	1.00	41.70	6
ATOM	641	OD1	ASN	909	14.196	39.684	8.168	1.00	41.70	8
ATOM	642	ND2	ASN	909	13.381	37.931	9.316	1.00	41.70	7
ATOM	643	C	ASN	909	11.488	36.349	7.964	1.00	31.42	6
ATOM	644	O	ASN	909	11.094	36.340	9.132	1.00	31.42	8
ATOM	645	N	LEU	910	11.937	35.275	7.347	1.00	17.12	7
ATOM	646	CA	LEU	910	11.930	34.014	8.019	1.00	17.12	6
ATOM	647	CB	LEU	910	12.524	32.962	7.139	1.00	20.29	6
ATOM	648	CG	LEU	910	12.192	31.558	7.604	1.00	20.29	6
ATOM	649	CD1	LEU	910	10.687	31.274	7.677	1.00	20.29	6
ATOM	650	CD2	LEU	910	12.850	30.696	6.590	1.00	20.29	6
ATOM	651	C	LEU	910	12.679	34.039	9.333	1.00	17.12	6
ATOM	652	O	LEU	910	12.183	33.554	10.355	1.00	17.12	8
ATOM	653	N	LEU	911	13.885	34.579	9.319	1.00	21.04	7
ATOM	654	CA	LEU	911	14.646	34.644	10.551	1.00	21.04	6
ATOM	655	CB	LEU	911	15.865	35.523	10.363	1.00	23.99	6
ATOM	656	CG	LEU	911	16.744	35.463	11.596	1.00	23.99	6
ATOM	657	CD1	LEU	911	17.326	34.053	11.797	1.00	23.99	6
ATOM	658	CD2	LEU	911	17.833	36.483	11.399	1.00	23.99	6
ATOM	659	C	LEU	911	13.791	35.199	11.697	1.00	21.04	6
ATOM	660	O	LEU	911	13.565	34.515	12.692	1.00	21.04	8
ATOM	661	N	ASP	912	13.305	36.429	11.557	1.00	16.81	7
ATOM	662	CA	ASP	912	12.489	37.041	12.618	1.00	16.81	6
ATOM	663	CB	ASP	912	11.973	38.399	12.177	1.00	39.39	6
ATOM	664	CG	ASP	912	12.996	39.463	12.327	1.00	39.39	6
ATOM	665	OD1	ASP	912	12.794	40.557	11.777	1.00	39.39	8
ATOM	666	OD2	ASP	912	14.005	39.185	12.989	1.00	39.39	8
ATOM	667	C	ASP	912	11.311	36.214	13.031	1.00	16.81	6
ATOM	668	O	ASP	912	11.020	36.079	14.215	1.00	16.81	8
ATOM	669	N	PHE	913	10.623	35.698	12.027	1.00	39.11	7
ATOM	670	CA	PHE	913	9.462	34.884	12.255	1.00	39.11	6
ATOM	671	CB	PHE	913	8.850	34.495	10.937	1.00	34.21	6
ATOM	672	CG	PHE	913	7.458	34.005	11.055	1.00	34.21	6
ATOM	673	CD1	PHE	913	6.412	34.897	11.233	1.00	34.21	6

FIG. 3L

ATOM	674	CD2	PHE	913	7.181	32.647	10.986	1.00	34.21	6
ATOM	675	CE1	PHE	913	5.109	34.450	11.343	1.00	34.21	6
ATOM	676	CE2	PHE	913	5.885	32.185	11.094	1.00	34.21	6
ATOM	677	CZ	PHE	913	4.843	33.089	11.271	1.00	34.21	6
ATOM	678	C	PHE	913	9.846	33.636	13.026	1.00	39.11	6
ATOM	679	O	PHE	913	9.073	33.166	13.843	1.00	39.11	8
ATOM	680	N	LEU	914	11.018	33.076	12.770	1.00	29.14	7
ATOM	681	CA	LEU	914	11.389	31.895	13.527	1.00	29.14	6
ATOM	682	CB	LEU	914	12.622	31.212	12.916	1.00	10.91	6
ATOM	683	CG	LEU	914	12.407	30.445	11.606	1.00	10.91	6
ATOM	684	CD1	LEU	914	13.709	29.936	11.066	1.00	10.91	6
ATOM	685	CD2	LEU	914	11.430	29.310	11.861	1.00	10.91	6
ATOM	686	C	LEU	914	11.659	32.247	14.994	1.00	29.14	6
ATOM	687	O	LEU	914	11.215	31.551	15.893	1.00	29.14	8
ATOM	688	N	ARG	915	12.377	33.337	15.228	1.00	18.56	7
ATOM	689	CA	ARG	915	12.750	33.766	16.569	1.00	18.56	6
ATOM	690	CB	ARG	915	13.829	34.844	16.463	1.00	29.12	6
ATOM	691	CG	ARG	915	15.088	34.300	15.887	1.00	29.12	6
ATOM	692	CD	ARG	915	16.140	35.354	15.729	1.00	29.12	6
ATOM	693	NE	ARG	915	17.459	34.736	15.660	1.00	29.12	7
ATOM	694	CZ	ARG	915	18.580	35.352	15.285	1.00	29.12	6
ATOM	695	NH1	ARG	915	18.545	36.630	14.924	1.00	29.12	7
ATOM	696	NH2	ARG	915	19.745	34.689	15.287	1.00	29.12	7
ATOM	697	C	ARG	915	11.609	34.256	17.439	1.00	18.56	6
ATOM	698	O	ARG	915	11.641	34.094	18.665	1.00	18.56	8
ATOM	699	N	LYS	916	10.605	34.841	16.788	1.00	22.66	7
ATOM	700	CA	LYS	916	9.426	35.406	17.441	1.00	22.66	6
ATOM	701	CB	LYS	916	8.816	36.463	16.501	1.00	51.60	6
ATOM	702	CG	LYS	916	7.369	36.228	16.021	1.00	51.60	6
ATOM	703	CD	LYS	916	7.163	34.999	15.123	1.00	51.60	6
ATOM	704	CE	LYS	916	5.699	34.865	14.684	1.00	51.60	6
ATOM	705	NZ	LYS	916	4.772	34.565	15.811	1.00	51.60	7
ATOM	706	C	LYS	916	8.377	34.360	17.848	1.00	22.66	6
ATOM	707	O	LYS	916	7.332	34.718	18.366	1.00	22.66	8
ATOM	708	N	SER	917	8.677	33.082	17.633	1.00	22.66	7
ATOM	709	CA	SER	917	7.773	31.979	17.957	1.00	22.66	6
ATOM	710	CB	SER	917	7.623	31.070	16.741	1.00	19.58	6
ATOM	711	OG	SER	917	8.890	30.564	16.328	1.00	19.58	8
ATOM	712	C	SER	917	8.272	31.143	19.135	1.00	22.66	6
ATOM	713	O	SER	917	7.720	30.078	19.436	1.00	22.66	8
ATOM	714	N	ARG	918	9.339	31.602	19.780	1.00	32.97	7
ATOM	715	CA	ARG	918	9.906	30.908	20.934	1.00	32.97	6
ATOM	716	CB	ARG	918	11.372	31.305	21.132	1.00	9.93	6
ATOM	717	CG	ARG	918	12.287	31.089	19.973	1.00	9.93	6
ATOM	718	CD	ARG	918	13.751	31.230	20.402	1.00	9.93	6
ATOM	719	NE	ARG	918	14.633	30.604	19.413	1.00	9.93	7
ATOM	720	CZ	ARG	918	15.957	30.509	19.504	1.00	9.93	6
ATOM	721	NH1	ARG	918	16.610	31.007	20.533	1.00	9.93	7
ATOM	722	NH2	ARG	918	16.637	29.872	18.565	1.00	9.93	7
ATOM	723	C	ARG	918	9.110	31.323	22.177	1.00	32.97	6
ATOM	724	O	ARG	918	9.547	32.189	22.925	1.00	32.97	8
ATOM	725	N	VAL	919	7.943	30.704	22.365	1.00	29.42	7
ATOM	726	CA	VAL	919	7.026	30.973	23.484	1.00	29.42	6
ATOM	727	CB	VAL	919	5.878	29.970	23.518	1.00	31.60	6
ATOM	728	CG1	VAL	919	4.650	30.613	24.113	1.00	31.60	6
ATOM	729	CG2	VAL	919	5.620	29.426	22.134	1.00	31.60	6
ATOM	730	C	VAL	919	7.635	30.893	24.867	1.00	29.42	6

FIG. 3M

ATOM	731	O	VAL	919	7.173	31.537	25.793	1.00	29.42	8
ATOM	732	N	LEU	920	8.635	30.048	25.020	1.00	34.37	7
ATOM	733	CA	LEU	920	9.260	29.900	26.305	1.00	34.37	6
ATOM	734	CB	LEU	920	10.093	28.629	26.324	1.00	36.03	6
ATOM	735	CG	LEU	920	10.688	28.310	27.688	1.00	36.03	6
ATOM	736	CD1	LEU	920	9.559	28.061	28.676	1.00	36.03	6
ATOM	737	CD2	LEU	920	11.592	27.104	27.587	1.00	36.03	6
ATOM	738	C	LEU	920	10.138	31.117	26.552	1.00	34.37	6
ATOM	739	O	LEU	920	10.523	31.393	27.676	1.00	34.37	8
ATOM	740	N	GLU	921	10.472	31.851	25.503	1.00	29.12	7
ATOM	741	CA	GLU	921	11.301	33.025	25.693	1.00	29.12	6
ATOM	742	CB	GLU	921	12.215	33.237	24.485	1.00	99.98	6
ATOM	743	CG	GLU	921	13.435	34.081	24.798	1.00	99.98	6
ATOM	744	CD	GLU	921	13.165	35.574	24.753	1.00	99.98	6
ATOM	745	OE1	GLU	921	12.935	36.086	23.638	1.00	99.98	8
ATOM	746	OE2	GLU	921	13.156	36.228	25.824	1.00	99.98	8
ATOM	747	C	GLU	921	10.362	34.207	25.885	1.00	29.12	6
ATOM	748	O	GLU	921	10.452	34.929	26.869	1.00	29.12	8
ATOM	749	N	THR	922	9.455	34.375	24.932	1.00	52.74	7
ATOM	750	CA	THR	922	8.463	35.437	24.944	1.00	52.74	6
ATOM	751	CB	THR	922	7.450	35.207	23.800	1.00	53.34	6
ATOM	752	OG1	THR	922	8.038	35.598	22.558	1.00	53.34	8
ATOM	753	CG2	THR	922	6.167	35.977	24.026	1.00	53.34	6
ATOM	754	C	THR	922	7.706	35.498	26.265	1.00	52.74	6
ATOM	755	O	THR	922	7.923	36.398	27.077	1.00	52.74	8
ATOM	756	N	ASP	923	6.827	34.515	26.461	1.00	32.25	7
ATOM	757	CA	ASP	923	5.981	34.391	27.651	1.00	32.25	6
ATOM	758	CB	ASP	923	4.509	34.434	27.231	1.00	60.93	6
ATOM	759	CG	ASP	923	3.558	34.328	28.404	1.00	60.93	6
ATOM	760	OD1	ASP	923	3.762	35.032	29.415	1.00	60.93	8
ATOM	761	OD2	ASP	923	2.593	33.545	28.309	1.00	60.93	8
ATOM	762	C	ASP	923	6.295	33.083	28.361	1.00	32.25	6
ATOM	763	O	ASP	923	5.711	32.034	28.055	1.00	32.25	8
ATOM	764	N	PRO	924	7.216	33.146	29.346	1.00	33.34	7
ATOM	765	CD	PRO	924	7.426	34.381	30.130	1.00	100.00	6
ATOM	766	CA	PRO	924	7.637	31.978	30.125	1.00	33.34	6
ATOM	767	CB	PRO	924	8.263	32.605	31.366	1.00	100.00	6
ATOM	768	CG	PRO	924	7.488	33.863	31.535	1.00	100.00	6
ATOM	769	C	PRO	924	6.464	31.030	30.456	1.00	33.34	6
ATOM	770	O	PRO	924	6.470	29.873	30.053	1.00	33.34	8
ATOM	771	N	ALA	925	5.460	31.543	31.164	1.00	69.10	7
ATOM	772	CA	ALA	925	4.282	30.781	31.603	1.00	69.10	6
ATOM	773	CB	ALA	925	3.311	31.735	32.255	1.00	73.73	6
ATOM	774	C	ALA	925	3.562	29.976	30.531	1.00	69.10	6
ATOM	775	O	ALA	925	3.802	28.779	30.384	1.00	69.10	8
ATOM	776	N	PHE	926	2.662	30.639	29.806	1.00	48.64	7
ATOM	777	CA	PHE	926	1.877	30.013	28.743	1.00	48.64	6
ATOM	778	CB	PHE	926	1.766	30.975	27.558	1.00	37.88	6
ATOM	779	CG	PHE	926	0.669	30.632	26.605	1.00	37.88	6
ATOM	780	CD1	PHE	926	-0.646	30.983	26.893	1.00	37.88	6
ATOM	781	CD2	PHE	926	0.926	29.853	25.479	1.00	37.88	6
ATOM	782	CE1	PHE	926	-1.679	30.560	26.089	1.00	37.88	6
ATOM	783	CE2	PHE	926	-0.106	29.420	24.668	1.00	37.88	6
ATOM	784	CZ	PHE	926	-1.406	29.774	24.977	1.00	37.88	6
ATOM	785	C	PHE	926	2.439	28.673	28.267	1.00	48.64	6
ATOM	786	O	PHE	926	1.752	27.656	28.298	1.00	48.64	8
ATOM	787	N	ALA	927	3.688	28.681	27.812	1.00	47.80	7

FIG. 3N

ATOM	788	CA	ALA	927	4.337	27.467	27.340	1.00 47.80	6
ATOM	789	CB	ALA	927	5.786	27.752	26.970	1.00 31.97	6
ATOM	790	C	ALA	927	4.272	26.297	28.314	1.00 47.80	6
ATOM	791	O	ALA	927	3.725	25.256	27.984	1.00 47.80	8
ATOM	792	N	ILE	928	4.850	26.439	29.499	1.00 44.35	7
ATOM	793	CA	ILE	928	4.810	25.346	30.457	1.00 44.35	6
ATOM	794	CB	ILE	928	5.155	25.837	31.868	1.00 67.81	6
ATOM	795	CG2	ILE	928	5.834	24.735	32.641	1.00 29.96	6
ATOM	796	CG1	ILE	928	6.130	27.004	31.806	1.00 29.96	6
ATOM	797	CD1	ILE	928	7.542	26.594	31.485	1.00 29.96	6
ATOM	798	C	ILE	928	3.410	24.718	30.494	1.00 44.35	6
ATOM	799	O	ILE	928	3.266	23.499	30.626	1.00 44.35	8
ATOM	800	N	ALA	929	2.390	25.562	30.346	1.00 42.29	7
ATOM	801	CA	ALA	929	0.984	25.135	30.390	1.00 42.29	6
ATOM	802	CB	ALA	929	0.118	26.315	30.676	1.00 5.26	6
ATOM	803	C	ALA	929	0.457	24.440	29.156	1.00 42.29	6
ATOM	804	O	ALA	929	-0.225	23.429	29.252	1.00 42.29	8
ATOM	805	N	ASN	930	0.745	24.995	27.994	1.00 36.17	7
ATOM	806	CA	ASN	930	0.259	24.398	26.775	1.00 36.17	6
ATOM	807	CB	ASN	930	-0.230	25.506	25.852	1.00 57.20	6
ATOM	808	CG	ASN	930	-1.444	26.223	26.430	1.00 57.20	6
ATOM	809	OD1	ASN	930	-2.586	25.742	26.344	1.00 57.20	8
ATOM	810	ND2	ASN	930	-1.202	27.360	27.057	1.00 57.20	7
ATOM	811	C	ASN	930	1.295	23.486	26.128	1.00 36.17	6
ATOM	812	O	ASN	930	1.088	22.976	25.028	1.00 36.17	8
ATOM	813	N	SER	931	2.401	23.259	26.834	1.00 50.28	7
ATOM	814	CA	SER	931	3.468	22.383	26.353	1.00 50.28	6
ATOM	815	CB	SER	931	2.986	20.930	26.341	1.00 90.81	6
ATOM	816	OG	SER	931	2.790	20.433	27.659	1.00 90.81	8
ATOM	817	C	SER	931	4.006	22.748	24.979	1.00 50.28	6
ATOM	818	O	SER	931	4.484	21.889	24.258	1.00 50.28	8
ATOM	819	N	THR	932	3.918	24.023	24.622	1.00 48.32	7
ATOM	820	CA	THR	932	4.397	24.510	23.334	1.00 48.32	6
ATOM	821	CB	THR	932	3.443	25.591	22.749	1.00 79.61	6
ATOM	822	OG1	THR	932	3.247	26.634	23.711	1.00 79.61	8
ATOM	823	CG2	THR	932	2.108	24.989	22.374	1.00 79.61	6
ATOM	824	C	THR	932	5.784	25.127	23.483	1.00 48.32	6
ATOM	825	O	THR	932	6.046	25.841	24.449	1.00 48.32	8
ATOM	826	N	ALA	933	6.667	24.854	22.527	1.00 55.05	7
ATOM	827	CA	ALA	933	8.009	25.436	22.552	1.00 55.05	6
ATOM	828	CB	ALA	933	9.057	24.378	22.297	1.00 28.55	6
ATOM	829	C	ALA	933	8.051	26.489	21.461	1.00 55.05	6
ATOM	830	O	ALA	933	8.936	27.339	21.437	1.00 55.05	8
ATOM	831	N	SER	934	7.098	26.393	20.543	1.00 27.13	7
ATOM	832	CA	SER	934	6.978	27.340	19.469	1.00 27.13	6
ATOM	833	CB	SER	934	7.937	27.003	18.341	1.00 36.98	6
ATOM	834	OG	SER	934	7.630	27.748	17.167	1.00 36.98	8
ATOM	835	C	SER	934	5.552	27.315	18.959	1.00 27.13	6
ATOM	836	O	SER	934	4.897	26.270	19.001	1.00 27.13	8
ATOM	837	N	THR	935	5.080	28.468	18.488	1.00 15.04	7
ATOM	838	CA	THR	935	3.740	28.582	17.963	1.00 15.04	6
ATOM	839	CB	THR	935	3.387	30.101	17.642	1.00 26.85	6
ATOM	840	OG1	THR	935	4.301	30.658	16.680	1.00 26.85	8
ATOM	841	CG2	THR	935	3.432	30.930	18.917	1.00 26.85	6
ATOM	842	C	THR	935	3.652	27.696	16.712	1.00 15.04	6
ATOM	843	O	THR	935	2.594	27.154	16.407	1.00 15.04	8
ATOM	844	N	LEU	936	4.778	27.530	16.015	1.00 41.56	7

FIG. 30

ATOM	845	CA	LEU	936	4.839	26.720	14.788	1.00	41.56	6
ATOM	846	CB	LEU	936	6.005	27.210	13.915	1.00	16.11	6
ATOM	847	CG	LEU	936	5.980	28.713	13.613	1.00	16.11	6
ATOM	848	CD1	LEU	936	7.108	29.067	12.679	1.00	16.11	6
ATOM	849	CD2	LEU	936	4.640	29.083	13.020	1.00	16.11	6
ATOM	850	C	LEU	936	4.958	25.203	15.018	1.00	41.56	6
ATOM	851	O	LEU	936	5.433	24.744	16.063	1.00	41.56	8
ATOM	852	N	SER	937	4.524	24.440	14.021	1.00	27.35	7
ATOM	853	CA	SER	937	4.551	22.989	14.081	1.00	27.35	6
ATOM	854	CB	SER	937	3.167	22.438	13.764	1.00	9.94	6
ATOM	855	OG	SER	937	2.884	22.429	12.374	1.00	9.94	8
ATOM	856	C	SER	937	5.574	22.357	13.128	1.00	27.35	6
ATOM	857	O	SER	937	6.180	23.041	12.291	1.00	27.35	8
ATOM	858	N	SER	938	5.752	21.043	13.257	1.00	23.83	7
ATOM	859	CA	SER	938	6.689	20.294	12.431	1.00	23.83	6
ATOM	860	CB	SER	938	6.678	18.813	12.838	1.00	31.90	6
ATOM	861	OG	SER	938	7.011	17.966	11.741	1.00	31.90	8
ATOM	862	C	SER	938	6.362	20.431	10.943	1.00	23.83	6
ATOM	863	O	SER	938	7.256	20.590	10.121	1.00	23.83	8
ATOM	864	N	GLN	939	5.083	20.382	10.597	1.00	34.70	7
ATOM	865	CA	GLN	939	4.704	20.491	9.206	1.00	34.70	6
ATOM	866	CB	GLN	939	3.296	19.955	9.022	1.00	40.81	6
ATOM	867	CG	GLN	939	3.189	18.544	9.538	1.00	40.81	6
ATOM	868	CD	GLN	939	4.026	17.558	8.732	1.00	40.81	6
ATOM	869	OE1	GLN	939	3.584	17.084	7.675	1.00	40.81	8
ATOM	870	NE2	GLN	939	5.243	17.254	9.216	1.00	40.81	7
ATOM	871	C	GLN	939	4.838	21.906	8.685	1.00	34.70	6
ATOM	872	O	GLN	939	5.352	22.096	7.592	1.00	34.70	8
ATOM	873	N	GLN	940	4.388	22.906	9.435	1.00	22.70	7
ATOM	874	CA	GLN	940	4.556	24.267	8.950	1.00	22.70	6
ATOM	875	CB	GLN	940	4.094	25.286	9.986	1.00	30.92	6
ATOM	876	CG	GLN	940	4.588	26.679	9.679	1.00	30.92	6
ATOM	877	CD	GLN	940	3.663	27.483	8.790	1.00	30.92	6
ATOM	878	OE1	GLN	940	2.738	28.141	9.277	1.00	30.92	8
ATOM	879	NE2	GLN	940	3.891	27.427	7.482	1.00	30.92	7
ATOM	880	C	GLN	940	6.047	24.501	8.632	1.00	22.70	6
ATOM	881	O	GLN	940	6.381	25.050	7.574	1.00	22.70	8
ATOM	882	N	LEU	941	6.934	24.076	9.535	1.00	22.33	7
ATOM	883	CA	LEU	941	8.377	24.242	9.348	1.00	22.33	6
ATOM	884	CB	LEU	941	9.137	23.858	10.599	1.00	19.37	6
ATOM	885	CG	LEU	941	8.939	24.738	11.806	1.00	19.37	6
ATOM	886	CD1	LEU	941	9.540	23.981	12.995	1.00	19.37	6
ATOM	887	CD2	LEU	941	9.613	26.094	11.606	1.00	19.37	6
ATOM	888	C	LEU	941	8.956	23.427	8.202	1.00	22.33	6
ATOM	889	O	LEU	941	9.994	23.781	7.648	1.00	22.33	8
ATOM	890	N	LEU	942	8.334	22.308	7.869	1.00	30.49	7
ATOM	891	CA	LEU	942	8.877	21.545	6.765	1.00	30.49	6
ATOM	892	CB	LEU	942	8.370	20.098	6.748	1.00	27.17	6
ATOM	893	CG	LEU	942	8.901	19.138	7.816	1.00	27.17	6
ATOM	894	CD1	LEU	942	8.244	17.799	7.576	1.00	27.17	6
ATOM	895	CD2	LEU	942	10.399	18.997	7.776	1.00	27.17	6
ATOM	896	C	LEU	942	8.445	22.285	5.517	1.00	30.49	6
ATOM	897	O	LEU	942	9.211	22.408	4.582	1.00	30.49	8
ATOM	898	N	HIS	943	7.224	22.805	5.502	1.00	24.87	7
ATOM	899	CA	HIS	943	6.766	23.543	4.331	1.00	24.87	6
ATOM	900	CB	HIS	943	5.393	24.127	4.565	1.00	75.69	6
ATOM	901	CG	HIS	943	4.306	23.142	4.316	1.00	75.69	6

FIG. 3P

ATOM	902	CD2	HIS	943	3.224	23.187	3.507	1.00	75.69	6
ATOM	903	ND1	HIS	943	4.317	21.892	4.884	1.00	75.69	7
ATOM	904	CE1	HIS	943	3.284	21.198	4.431	1.00	75.69	6
ATOM	905	NE2	HIS	943	2.608	21.960	3.596	1.00	75.69	7
ATOM	906	C	HIS	943	7.727	24.644	3.967	1.00	24.87	6
ATOM	907	O	HIS	943	8.112	24.794	2.815	1.00	24.87	8
ATOM	908	N	PHE	944	8.107	25.412	4.976	1.00	23.28	7
ATOM	909	CA	PHE	944	9.049	26.499	4.812	1.00	23.28	6
ATOM	910	CB	PHE	944	9.379	27.069	6.196	1.00	24.44	6
ATOM	911	CG	PHE	944	8.293	27.953	6.782	1.00	24.44	6
ATOM	912	CD1	PHE	944	8.361	28.370	8.101	1.00	24.44	6
ATOM	913	CD2	PHE	944	7.282	28.477	5.983	1.00	24.44	6
ATOM	914	CE1	PHE	944	7.449	29.299	8.598	1.00	24.44	6
ATOM	915	CE2	PHE	944	6.372	29.406	6.489	1.00	24.44	6
ATOM	916	CZ	PHE	944	6.466	29.815	7.792	1.00	24.44	6
ATOM	917	C	PHE	944	10.301	26.011	4.079	1.00	23.28	6
ATOM	918	O	PHE	944	10.778	26.675	3.164	1.00	23.28	8
ATOM	919	N	ALA	945	10.829	24.855	4.470	1.00	15.27	7
ATOM	920	CA	ALA	945	11.996	24.310	3.799	1.00	15.27	6
ATOM	921	CB	ALA	945	12.627	23.197	4.645	1.00	55.81	6
ATOM	922	C	ALA	945	11.644	23.804	2.386	1.00	15.27	6
ATOM	923	O	ALA	945	12.493	23.819	1.517	1.00	15.27	8
ATOM	924	N	ALA	946	10.408	23.368	2.139	1.00	9.68	7
ATOM	925	CA	ALA	946	10.011	22.897	0.795	1.00	9.68	6
ATOM	926	CB	ALA	946	8.734	22.042	0.869	1.00	20.69	6
ATOM	927	C	ALA	946	9.760	24.088	-0.114	1.00	9.68	6
ATOM	928	O	ALA	946	10.026	24.032	-1.319	1.00	9.68	8
ATOM	929	N	ASP	947	9.205	25.149	0.471	1.00	24.26	7
ATOM	930	CA	ASP	947	8.922	26.379	-0.245	1.00	24.26	6
ATOM	931	CB	ASP	947	8.300	27.430	0.671	1.00	51.33	6
ATOM	932	CG	ASP	947	6.870	27.122	1.021	1.00	51.33	6
ATOM	933	OD1	ASP	947	6.378	26.066	0.572	1.00	51.33	8
ATOM	934	OD2	ASP	947	6.248	27.934	1.740	1.00	51.33	8
ATOM	935	C	ASP	947	10.231	26.909	-0.772	1.00	24.26	6
ATOM	936	O	ASP	947	10.378	27.109	-1.979	1.00	24.26	8
ATOM	937	N	VAL	948	11.192	27.120	0.123	1.00	17.83	7
ATOM	938	CA	VAL	948	12.458	27.641	-0.335	1.00	17.83	6
ATOM	939	CB	VAL	948	13.483	27.833	0.788	1.00	5.04	6
ATOM	940	CG1	VAL	948	14.786	28.296	0.175	1.00	5.04	6
ATOM	941	CG2	VAL	948	13.012	28.856	1.801	1.00	5.04	6
ATOM	942	C	VAL	948	13.078	26.766	-1.412	1.00	17.83	6
ATOM	943	O	VAL	948	13.514	27.304	-2.425	1.00	17.83	8
ATOM	944	N	ALA	949	13.115	25.442	-1.219	1.00	24.98	7
ATOM	945	CA	ALA	949	13.697	24.531	-2.221	1.00	24.98	6
ATOM	946	CB	ALA	949	13.827	23.129	-1.666	1.00	53.47	6
ATOM	947	C	ALA	949	12.882	24.505	-3.505	1.00	24.98	6
ATOM	948	O	ALA	949	13.440	24.313	-4.576	1.00	24.98	8
ATOM	949	N	ARG	950	11.570	24.716	-3.413	1.00	23.96	7
ATOM	950	CA	ARG	950	10.742	24.733	-4.617	1.00	23.96	6
ATOM	951	CB	ARG	950	9.239	24.736	-4.282	1.00	30.38	6
ATOM	952	CG	ARG	950	8.302	24.244	-5.419	1.00	30.38	6
ATOM	953	CD	ARG	950	6.829	24.454	-5.081	1.00	30.38	6
ATOM	954	NE	ARG	950	6.567	24.306	-3.648	1.00	30.38	7
ATOM	955	CZ	ARG	950	6.313	23.154	-3.030	1.00	30.38	6
ATOM	956	NH1	ARG	950	6.270	22.013	-3.723	1.00	30.38	7
ATOM	957	NH2	ARG	950	6.132	23.146	-1.708	1.00	30.38	7
ATOM	958	C	ARG	950	11.091	25.997	-5.391	1.00	23.96	6

FIG. 3Q

ATOM	959	O	ARG	950	11.089	26.003	-6.617	1.00	23.96	8
ATOM	960	N	GLY	951	11.409	27.064	-4.667	1.00	35.74	7
ATOM	961	CA	GLY	951	11.749	28.315	-5.323	1.00	35.74	6
ATOM	962	C	GLY	951	13.156	28.338	-5.890	1.00	35.74	6
ATOM	963	O	GLY	951	13.439	29.046	-6.850	1.00	35.74	8
ATOM	964	N	MET	952	14.050	27.562	-5.294	1.00	35.49	7
ATOM	965	CA	MET	952	15.430	27.512	-5.755	1.00	35.49	6
ATOM	966	CB	MET	952	16.335	26.979	-4.656	1.00	28.83	6
ATOM	967	CG	MET	952	16.616	27.981	-3.562	1.00	28.83	6
ATOM	968	SD	MET	952	17.396	29.511	-4.180	1.00	28.83	16
ATOM	969	CE	MET	952	18.963	28.883	-4.732	1.00	28.83	6
ATOM	970	C	MET	952	15.553	26.645	-6.972	1.00	35.49	6
ATOM	971	O	MET	952	16.480	26.786	-7.759	1.00	35.49	8
ATOM	972	N	ASP	953	14.623	25.723	-7.119	1.00	22.04	7
ATOM	973	CA	ASP	953	14.658	24.863	-8.277	1.00	22.04	6
ATOM	974	CB	ASP	953	13.701	23.708	-8.065	1.00	46.74	6
ATOM	975	CG	ASP	953	13.868	22.649	-9.095	1.00	46.74	6
ATOM	976	OD1	ASP	953	14.938	22.016	-9.119	1.00	46.74	8
ATOM	977	OD2	ASP	953	12.934	22.479	-9.894	1.00	46.74	8
ATOM	978	C	ASP	953	14.285	25.650	-9.534	1.00	22.04	6
ATOM	979	O	ASP	953	14.796	25.378	-10.600	1.00	22.04	8
ATOM	980	N	TYR	954	13.388	26.620	-9.391	1.00	30.73	7
ATOM	981	CA	TYR	954	12.969	27.454	-10.506	1.00	30.73	6
ATOM	982	CB	TYR	954	11.735	28.261	-10.120	1.00	46.88	6
ATOM	983	CG	TYR	954	11.212	29.222	-11.180	1.00	46.88	6
ATOM	984	CD1	TYR	954	10.358	28.777	-12.198	1.00	46.88	6
ATOM	985	CE1	TYR	954	9.817	29.675	-13.139	1.00	46.88	6
ATOM	986	CD2	TYR	954	11.523	30.596	-11.131	1.00	46.88	6
ATOM	987	CE2	TYR	954	10.987	31.498	-12.071	1.00	46.88	6
ATOM	988	CZ	TYR	954	10.139	31.023	-13.062	1.00	46.88	6
ATOM	989	OH	TYR	954	9.618	31.893	-13.980	1.00	46.88	8
ATOM	990	C	TYR	954	14.104	28.406	-10.820	1.00	30.73	6
ATOM	991	O	TYR	954	14.484	28.556	-11.961	1.00	30.73	8
ATOM	992	N	LEU	955	14.654	29.048	-9.801	1.00	22.51	7
ATOM	993	CA	LEU	955	15.727	29.991	-10.043	1.00	22.51	6
ATOM	994	CB	LEU	955	16.100	30.747	-8.771	1.00	36.85	6
ATOM	995	CG	LEU	955	15.064	31.599	-8.184	1.00	36.85	6
ATOM	996	CD1	LEU	955	15.708	32.365	-7.021	1.00	36.85	6
ATOM	997	CD2	LEU	955	14.586	32.734	-9.210	1.00	36.85	6
ATOM	998	C	LEU	955	16.963	29.355	-10.619	1.00	22.51	6
ATOM	999	O	LEU	955	17.530	29.885	-11.560	1.00	22.51	8
ATOM	1000	N	SER	956	17.403	28.229	-10.080	1.00	31.05	7
ATOM	1001	CA	SER	956	18.608	27.602	-10.615	1.00	31.05	6
ATOM	1002	CB	SER	956	18.998	26.380	-9.778	1.00	57.17	6
ATOM	1003	OG	SER	956	18.077	25.324	-9.989	1.00	57.17	8
ATOM	1004	C	SER	956	18.439	27.207	-12.084	1.00	31.05	6
ATOM	1005	O	SER	956	19.379	27.348	-12.858	1.00	31.05	8
ATOM	1006	N	GLN	957	17.247	26.732	-12.462	1.00	19.64	7
ATOM	1007	CA	GLN	957	16.932	26.307	-13.841	1.00	19.64	6
ATOM	1008	CB	GLN	957	15.580	25.587	-13.899	1.00	97.55	6
ATOM	1009	CG	GLN	957	15.565	24.175	-13.366	1.00	97.55	6
ATOM	1010	CD	GLN	957	16.884	23.460	-13.539	1.00	97.55	6
ATOM	1011	OE1	GLN	957	17.543	23.597	-14.568	1.00	97.55	8
ATOM	1012	NE2	GLN	957	17.275	22.679	-12.532	1.00	97.55	7
ATOM	1013	C	GLN	957	16.901	27.437	-14.860	1.00	19.64	6
ATOM	1014	O	GLN	957	16.903	27.191	-16.054	1.00	19.64	8
ATOM	1015	N	LYS	958	16.815	28.666	-14.370	1.00	37.82	7

FIG. 3R

ATOM	1016	CA	LYS	958	16.801	29.851	-15.205	1.00 37.82	6
ATOM	1017	CB	LYS	958	15.881	30.918	-14.601	1.00 51.85	6
ATOM	1018	CG	LYS	958	14.374	30.580	-14.569	1.00 51.85	6
ATOM	1019	CD	LYS	958	13.831	30.551	-15.986	1.00 51.85	6
ATOM	1020	CE	LYS	958	12.345	30.408	-16.083	1.00 51.85	6
ATOM	1021	NZ	LYS	958	12.076	30.168	-17.526	1.00 51.85	7
ATOM	1022	C	LYS	958	18.236	30.355	-15.192	1.00 37.82	6
ATOM	1023	O	LYS	958	18.528	31.466	-15.641	1.00 37.82	8
ATOM	1024	N	GLN	959	19.129	29.546	-14.634	1.00 37.14	7
ATOM	1025	CA	GLN	959	20.543	29.885	-14.550	1.00 37.14	6
ATOM	1026	CB	GLN	959	21.078	30.229	-15.942	1.00 59.23	6
ATOM	1027	CG	GLN	959	20.943	29.096	-16.925	1.00 59.23	6
ATOM	1028	CD	GLN	959	21.605	27.827	-16.441	1.00 59.23	6
ATOM	1029	OE1	GLN	959	22.832	27.742	-16.372	1.00 59.23	8
ATOM	1030	NE2	GLN	959	20.790	26.844	-16.047	1.00 59.23	7
ATOM	1031	C	GLN	959	20.914	31.004	-13.559	1.00 37.14	6
ATOM	1032	O	GLN	959	21.937	31.669	-13.751	1.00 37.14	8
ATOM	1033	N	PHE	960	20.097	31.201	-12.519	1.00 48.69	7
ATOM	1034	CA	PHE	960	20.369	32.208	-11.492	1.00 48.69	6
ATOM	1035	CB	PHE	960	19.067	32.712	-10.840	1.00 18.22	6
ATOM	1036	CG	PHE	960	18.261	33.647	-11.686	1.00 18.22	6
ATOM	1037	CD1	PHE	960	17.426	33.166	-12.686	1.00 18.22	6
ATOM	1038	CD2	PHE	960	18.343	35.023	-11.493	1.00 18.22	6
ATOM	1039	CE1	PHE	960	16.677	34.044	-13.502	1.00 18.22	6
ATOM	1040	CE2	PHE	960	17.607	35.908	-12.296	1.00 18.22	6
ATOM	1041	CZ	PHE	960	16.777	35.415	-13.301	1.00 18.22	6
ATOM	1042	C	PHE	960	21.225	31.549	-10.402	1.00 48.69	6
ATOM	1043	O	PHE	960	21.203	30.329	-10.251	1.00 48.69	8
ATOM	1044	N	ILE	961	22.000	32.348	-9.674	1.00 25.93	7
ATOM	1045	CA	ILE	961	22.814	31.840	-8.561	1.00 25.93	6
ATOM	1046	CB	ILE	961	24.347	31.827	-8.883	1.00 5.00	6
ATOM	1047	CG2	ILE	961	25.140	31.201	-7.756	1.00 5.00	6
ATOM	1048	CG1	ILE	961	24.610	31.048	-10.132	1.00 5.00	6
ATOM	1049	CD1	ILE	961	25.990	31.281	-10.676	1.00 5.00	6
ATOM	1050	C	ILE	961	22.542	32.864	-7.449	1.00 25.93	6
ATOM	1051	O	ILE	961	22.658	34.061	-7.689	1.00 25.93	8
ATOM	1052	N	HIS	962	22.193	32.412	-6.247	1.00 38.00	7
ATOM	1053	CA	HIS	962	21.871	33.355	-5.180	1.00 38.00	6
ATOM	1054	CB	HIS	962	21.093	32.661	-4.072	1.00 25.73	6
ATOM	1055	CG	HIS	962	20.206	33.579	-3.289	1.00 25.73	6
ATOM	1056	CD2	HIS	962	20.482	34.461	-2.308	1.00 25.73	6
ATOM	1057	ND1	HIS	962	18.846	33.614	-3.475	1.00 25.73	7
ATOM	1058	CE1	HIS	962	18.315	34.478	-2.625	1.00 25.73	6
ATOM	1059	NE2	HIS	962	19.282	35.004	-1.903	1.00 25.73	7
ATOM	1060	C	HIS	962	23.054	34.079	-4.573	1.00 38.00	6
ATOM	1061	O	HIS	962	23.119	35.303	-4.637	1.00 38.00	8
ATOM	1062	N	ARG	963	23.972	33.338	-3.958	1.00 61.33	7
ATOM	1063	CA	ARG	963	25.152	33.932	-3.334	1.00 61.33	6
ATOM	1064	CB	ARG	963	25.855	34.907	-4.306	1.00 42.94	6
ATOM	1065	CG	ARG	963	25.864	34.466	-5.753	1.00 42.94	6
ATOM	1066	CD	ARG	963	26.986	35.078	-6.571	1.00 42.94	6
ATOM	1067	NE	ARG	963	26.799	36.481	-6.929	1.00 42.94	7
ATOM	1068	CZ	ARG	963	26.940	37.488	-6.079	1.00 42.94	6
ATOM	1069	NH1	ARG	963	27.268	37.258	-4.809	1.00 42.94	7
ATOM	1070	NH2	ARG	963	26.752	38.723	-6.508	1.00 42.94	7
ATOM	1071	C	ARG	963	24.756	34.688	-2.062	1.00 61.33	6
ATOM	1072	O	ARG	963	25.543	35.464	-1.528	1.00 61.33	8

FIG. 3S

ATOM	1073	N	ASN	964	23.549	34.460	-1.561	1.00 37.36	7
ATOM	1074	CA	ASN	964	23.111	35.212	-0.384	1.00 37.36	6
ATOM	1075	CB	ASN	964	22.742	36.636	-0.805	1.00 69.75	6
ATOM	1076	CG	ASN	964	23.319	37.670	0.107	1.00 69.75	6
ATOM	1077	OD1	ASN	964	23.337	37.499	1.324	1.00 69.75	8
ATOM	1078	ND2	ASN	964	23.792	38.761	-0.468	1.00 69.75	7
ATOM	1079	C	ASN	964	21.909	34.573	0.273	1.00 37.36	6
ATOM	1080	O	ASN	964	21.096	35.251	0.890	1.00 37.36	8
ATOM	1081	N	LEU	965	21.812	33.258	0.133	1.00 45.72	7
ATOM	1082	CA	LEU	965	20.691	32.503	0.666	1.00 45.72	6
ATOM	1083	CB	LEU	965	20.515	31.230	-0.182	1.00 22.49	6
ATOM	1084	CG	LEU	965	19.348	30.261	-0.002	1.00 22.49	6
ATOM	1085	CD1	LEU	965	19.237	29.344	-1.189	1.00 22.49	6
ATOM	1086	CD2	LEU	965	19.565	29.461	1.252	1.00 22.49	6
ATOM	1087	C	LEU	965	20.867	32.180	2.151	1.00 45.72	6
ATOM	1088	O	LEU	965	21.862	31.584	2.564	1.00 45.72	8
ATOM	1089	N	ALA	966	19.898	32.605	2.948	1.00 9.29	7
ATOM	1090	CA	ALA	966	19.899	32.364	4.386	1.00 9.29	6
ATOM	1091	CB	ALA	966	20.870	33.291	5.057	1.00 5.00	6
ATOM	1092	C	ALA	966	18.474	32.615	4.891	1.00 9.29	6
ATOM	1093	O	ALA	966	17.613	32.963	4.107	1.00 9.29	8
ATOM	1094	N	ALA	967	18.209	32.464	6.181	1.00 20.93	7
ATOM	1095	CA	ALA	967	16.855	32.698	6.627	1.00 20.93	6
ATOM	1096	CB	ALA	967	16.627	32.084	7.989	1.00 8.30	6
ATOM	1097	C	ALA	967	16.481	34.170	6.630	1.00 20.93	6
ATOM	1098	O	ALA	967	15.335	34.486	6.393	1.00 20.93	8
ATOM	1099	N	ARG	968	17.423	35.077	6.875	1.00 18.97	7
ATOM	1100	CA	ARG	968	17.100	36.503	6.901	1.00 18.97	6
ATOM	1101	CB	ARG	968	18.298	37.322	7.381	1.00 55.21	6
ATOM	1102	CG	ARG	968	19.596	36.932	6.747	1.00 55.21	6
ATOM	1103	CD	ARG	968	20.653	38.006	6.946	1.00 55.21	6
ATOM	1104	NE	ARG	968	21.881	37.608	6.275	1.00 55.21	7
ATOM	1105	CZ	ARG	968	22.617	36.572	6.652	1.00 55.21	6
ATOM	1106	NH1	ARG	968	22.246	35.846	7.704	1.00 55.21	7
ATOM	1107	NH2	ARG	968	23.697	36.244	5.954	1.00 55.21	7
ATOM	1108	C	ARG	968	16.632	37.016	5.548	1.00 18.97	6
ATOM	1109	O	ARG	968	15.790	37.915	5.477	1.00 18.97	8
ATOM	1110	N	ASN	969	17.165	36.427	4.481	1.00 17.09	7
ATOM	1111	CA	ASN	969	16.820	36.815	3.109	1.00 17.09	6
ATOM	1112	CB	ASN	969	18.008	36.589	2.179	1.00 47.15	6
ATOM	1113	CG	ASN	969	19.028	37.700	2.240	1.00 47.15	6
ATOM	1114	OD1	ASN	969	20.137	37.547	1.739	1.00 47.15	8
ATOM	1115	ND2	ASN	969	18.661	38.831	2.842	1.00 47.15	7
ATOM	1116	C	ASN	969	15.619	36.088	2.526	1.00 17.09	6
ATOM	1117	O	ASN	969	15.524	35.926	1.318	1.00 17.09	8
ATOM	1118	N	ILE	970	14.725	35.625	3.385	1.00 17.16	7
ATOM	1119	CA	ILE	970	13.527	34.939	2.933	1.00 17.16	6
ATOM	1120	CB	ILE	970	13.521	33.425	3.353	1.00 5.00	6
ATOM	1121	CG2	ILE	970	12.211	32.763	2.943	1.00 5.00	6
ATOM	1122	CG1	ILE	970	14.716	32.686	2.742	1.00 5.00	6
ATOM	1123	CD1	ILE	970	14.542	32.175	1.313	1.00 5.00	6
ATOM	1124	C	ILE	970	12.395	35.687	3.653	1.00 17.16	6
ATOM	1125	O	ILE	970	12.454	35.923	4.864	1.00 17.16	8
ATOM	1126	N	LEU	971	11.365	36.047	2.903	1.00 27.06	7
ATOM	1127	CA	LEU	971	10.234	36.784	3.443	1.00 27.06	6
ATOM	1128	CB	LEU	971	10.000	38.039	2.584	1.00 23.00	6
ATOM	1129	CG	LEU	971	11.152	39.063	2.555	1.00 23.00	6

FIG. 3T

ATOM	1130	CD1	LEU	971	11.197	39.762	1.249	1.00	23.00	6
ATOM	1131	CD2	LEU	971	10.990	40.054	3.689	1.00	23.00	6
ATOM	1132	C	LEU	971	8.984	35.910	3.465	1.00	27.06	6
ATOM	1133	O	LEU	971	8.730	35.192	2.511	1.00	27.06	8
ATOM	1134	N	VAL	972	8.218	35.967	4.558	1.00	35.27	7
ATOM	1135	CA	VAL	972	6.974	35.188	4.710	1.00	35.27	6
ATOM	1136	CB	VAL	972	6.641	34.916	6.237	1.00	15.12	6
ATOM	1137	CG1	VAL	972	5.384	34.069	6.387	1.00	15.12	6
ATOM	1138	CG2	VAL	972	7.806	34.239	6.917	1.00	15.12	6
ATOM	1139	C	VAL	972	5.805	35.979	4.086	1.00	35.27	6
ATOM	1140	O	VAL	972	5.220	36.848	4.727	1.00	35.27	8
ATOM	1141	N	GLY	973	5.466	35.686	2.841	1.00	28.86	7
ATOM	1142	CA	GLY	973	4.378	36.404	2.212	1.00	28.86	6
ATOM	1143	C	GLY	973	3.021	35.983	2.743	1.00	28.86	6
ATOM	1144	O	GLY	973	2.933	35.251	3.734	1.00	28.86	8
ATOM	1145	N	GLU	974	1.954	36.429	2.092	1.00	36.97	7
ATOM	1146	CA	GLU	974	0.621	36.081	2.554	1.00	36.97	6
ATOM	1147	CB	GLU	974	-0.434	36.662	1.619	1.00	98.72	6
ATOM	1148	CG	GLU	974	-1.001	37.980	2.107	1.00	98.72	6
ATOM	1149	CD	GLU	974	-1.619	37.873	3.503	1.00	98.72	6
ATOM	1150	OE1	GLU	974	-2.364	36.904	3.759	1.00	98.72	8
ATOM	1151	OE2	GLU	974	-1.368	38.763	4.342	1.00	98.72	8
ATOM	1152	C	GLU	974	0.418	34.585	2.720	1.00	36.97	6
ATOM	1153	O	GLU	974	1.049	33.768	2.034	1.00	36.97	8
ATOM	1154	N	ASN	975	-0.474	34.253	3.649	1.00	50.17	7
ATOM	1155	CA	ASN	975	-0.811	32.878	3.980	1.00	50.17	6
ATOM	1156	CB	ASN	975	-1.496	32.190	2.812	1.00	49.51	6
ATOM	1157	CG	ASN	975	-2.900	32.725	2.577	1.00	49.51	6
ATOM	1158	OD1	ASN	975	-3.688	32.145	1.834	1.00	49.51	8
ATOM	1159	ND2	ASN	975	-3.218	33.851	3.213	1.00	49.51	7
ATOM	1160	C	ASN	975	0.432	32.122	4.392	1.00	50.17	6
ATOM	1161	O	ASN	975	0.528	30.910	4.222	1.00	50.17	8
ATOM	1162	N	TYR	976	1.386	32.871	4.931	1.00	34.67	7
ATOM	1163	CA	TYR	976	2.637	32.335	5.427	1.00	34.67	6
ATOM	1164	CB	TYR	976	2.386	31.613	6.734	1.00	32.84	6
ATOM	1165	CG	TYR	976	1.690	32.497	7.736	1.00	32.84	6
ATOM	1166	CD1	TYR	976	0.309	32.654	7.715	1.00	32.84	6
ATOM	1167	CE1	TYR	976	-0.328	33.464	8.625	1.00	32.84	6
ATOM	1168	CD2	TYR	976	2.411	33.182	8.693	1.00	32.84	6
ATOM	1169	CE2	TYR	976	1.792	33.991	9.602	1.00	32.84	6
ATOM	1170	CZ	TYR	976	0.422	34.129	9.571	1.00	32.84	6
ATOM	1171	OH	TYR	976	-0.210	34.897	10.515	1.00	32.84	8
ATOM	1172	C	TYR	976	3.376	31.440	4.475	1.00	34.67	6
ATOM	1173	O	TYR	976	3.903	30.410	4.875	1.00	34.67	8
ATOM	1174	N	VAL	977	3.436	31.857	3.217	1.00	16.20	7
ATOM	1175	CA	VAL	977	4.135	31.111	2.181	1.00	16.20	6
ATOM	1176	CB	VAL	977	3.297	31.091	0.876	1.00	9.07	6
ATOM	1177	CG1	VAL	977	4.187	30.767	-0.331	1.00	9.07	6
ATOM	1178	CG2	VAL	977	2.153	30.102	1.005	1.00	9.07	6
ATOM	1179	C	VAL	977	5.490	31.755	1.900	1.00	16.20	6
ATOM	1180	O	VAL	977	5.545	32.795	1.284	1.00	16.20	8
ATOM	1181	N	ALA	978	6.571	31.126	2.337	1.00	15.88	7
ATOM	1182	CA	ALA	978	7.924	31.643	2.141	1.00	15.88	6
ATOM	1183	CB	ALA	978	8.940	30.547	2.489	1.00	21.88	6
ATOM	1184	C	ALA	978	8.238	32.215	0.757	1.00	15.88	6
ATOM	1185	O	ALA	978	7.905	31.630	-0.268	1.00	15.88	8
ATOM	1186	N	LYS	979	8.920	33.352	0.736	1.00	28.57	7

FIG. 3U

ATOM	1187	CA	LYS	979	9.284	34.011	-0.508	1.00	28.57	6
ATOM	1188	CB	LYS	979	8.468	35.289	-0.621	1.00	15.51	6
ATOM	1189	CG	LYS	979	6.969	35.078	-0.838	1.00	15.51	6
ATOM	1190	CD	LYS	979	6.698	34.786	-2.297	1.00	15.51	6
ATOM	1191	CE	LYS	979	5.254	35.044	-2.662	1.00	15.51	6
ATOM	1192	NZ	LYS	979	4.388	34.606	-1.545	1.00	15.51	7
ATOM	1193	C	LYS	979	10.800	34.294	-0.506	1.00	28.57	6
ATOM	1194	O	LYS	979	11.348	34.679	0.525	1.00	28.57	8
ATOM	1195	N	ILE	980	11.458	34.082	-1.655	1.00	23.28	7
ATOM	1196	CA	ILE	980	12.914	34.271	-1.815	1.00	23.28	6
ATOM	1197	CB	ILE	980	13.507	33.236	-2.812	1.00	12.16	6
ATOM	1198	CG2	ILE	980	14.986	33.535	-3.046	1.00	12.16	6
ATOM	1199	CG1	ILE	980	13.309	31.804	-2.268	1.00	12.16	6
ATOM	1200	CD1	ILE	980	13.475	30.688	-3.319	1.00	12.16	6
ATOM	1201	C	ILE	980	13.270	35.665	-2.301	1.00	23.28	6
ATOM	1202	O	ILE	980	12.739	36.135	-3.292	1.00	23.28	8
ATOM	1203	N	ALA	981	14.185	36.335	-1.623	1.00	30.98	7
ATOM	1204	CA	ALA	981	14.538	37.683	-2.040	1.00	30.98	6
ATOM	1205	CB	ALA	981	13.810	38.664	-1.156	1.00	12.02	6
ATOM	1206	C	ALA	981	16.047	37.959	-2.021	1.00	30.98	6
ATOM	1207	O	ALA	981	16.840	37.172	-1.499	1.00	30.98	8
ATOM	1208	N	ASP	982	16.433	39.094	-2.589	1.00	70.73	7
ATOM	1209	CA	ASP	982	17.834	39.511	-2.652	1.00	70.73	6
ATOM	1210	CB	ASP	982	18.327	39.939	-1.272	1.00	99.58	6
ATOM	1211	CG	ASP	982	19.512	40.861	-1.358	1.00	99.58	6
ATOM	1212	OD1	ASP	982	19.287	42.012	-1.783	1.00	99.58	8
ATOM	1213	OD2	ASP	982	20.646	40.436	-1.039	1.00	99.58	8
ATOM	1214	C	ASP	982	18.821	38.488	-3.199	1.00	70.73	6
ATOM	1215	O	ASP	982	19.686	38.005	-2.477	1.00	70.73	8
ATOM	1216	N	PHE	983	18.703	38.184	-4.479	1.00	67.82	7
ATOM	1217	CA	PHE	983	19.595	37.229	-5.095	1.00	67.82	6
ATOM	1218	CB	PHE	983	18.781	36.124	-5.784	1.00	46.69	6
ATOM	1219	CG	PHE	983	17.480	36.593	-6.382	1.00	46.69	6
ATOM	1220	CD1	PHE	983	17.423	37.752	-7.143	1.00	46.69	6
ATOM	1221	CD2	PHE	983	16.317	35.852	-6.222	1.00	46.69	6
ATOM	1222	CE1	PHE	983	16.229	38.166	-7.737	1.00	46.69	6
ATOM	1223	CE2	PHE	983	15.122	36.259	-6.814	1.00	46.69	6
ATOM	1224	CZ	PHE	983	15.080	37.413	-7.570	1.00	46.69	6
ATOM	1225	C	PHE	983	20.552	37.905	-6.081	1.00	67.82	6
ATOM	1226	O	PHE	983	20.451	39.112	-6.338	1.00	67.82	8
ATOM	1227	N	GLY	984	21.497	37.128	-6.599	1.00	44.02	7
ATOM	1228	CA	GLY	984	22.467	37.644	-7.543	1.00	44.02	6
ATOM	1229	C	GLY	984	21.911	37.639	-8.954	1.00	44.02	6
ATOM	1230	O	GLY	984	21.520	36.599	-9.488	1.00	44.02	8
ATOM	1231	N	LEU	985	21.875	38.816	-9.562	1.00	100.00	7
ATOM	1232	CA	LEU	985	21.363	38.951	-10.917	1.00	100.00	6
ATOM	1233	CB	LEU	985	20.792	40.360	-11.126	1.00	41.04	6
ATOM	1234	CG	LEU	985	19.455	40.644	-10.434	1.00	41.04	6
ATOM	1235	CD1	LEU	985	18.448	39.621	-10.945	1.00	41.04	6
ATOM	1236	CD2	LEU	985	19.577	40.549	-8.925	1.00	41.04	6
ATOM	1237	C	LEU	985	22.473	38.670	-11.920	1.00	100.00	6
ATOM	1238	O	LEU	985	22.517	39.253	-13.004	1.00	100.00	8
ATOM	1239	N	SER	986	23.383	37.785	-11.539	1.00	42.70	7
ATOM	1240	CA	SER	986	24.484	37.421	-12.416	1.00	42.70	6
ATOM	1241	CB	SER	986	25.818	37.625	-11.697	1.00	68.70	6
ATOM	1242	OG	SER	986	25.996	38.984	-11.346	1.00	68.70	8
ATOM	1243	C	SER	986	24.295	35.955	-12.780	1.00	42.70	6

FIG. 3V

ATOM	1244	O	SER	986	24.956	35.078	-12.238	1.00 42.70	8
ATOM	1245	N	ARG	987	23.381	35.697	-13.703	1.00 47.12	7
ATOM	1246	CA	ARG	987	23.068	34.336	-14.124	1.00 47.12	6
ATOM	1247	CB	ARG	987	21.873	34.383	-15.045	1.00 55.43	6
ATOM	1248	CG	ARG	987	20.828	35.354	-14.585	1.00 55.43	6
ATOM	1249	CD	ARG	987	19.927	35.581	-15.728	1.00 55.43	6
ATOM	1250	NE	ARG	987	19.371	34.311	-16.169	1.00 55.43	7
ATOM	1251	CZ	ARG	987	18.891	34.116	-17.385	1.00 55.43	6
ATOM	1252	NH1	ARG	987	18.924	35.110	-18.261	1.00 55.43	7
ATOM	1253	NH2	ARG	987	18.364	32.946	-17.713	1.00 55.43	7
ATOM	1254	C	ARG	987	24.204	33.608	-14.823	1.00 47.12	6
ATOM	1255	O	ARG	987	24.990	34.223	-15.535	1.00 47.12	8
ATOM	1256	N	GLY	988	24.281	32.294	-14.629	1.00 32.39	7
ATOM	1257	CA	GLY	988	25.330	31.512	-15.274	1.00 32.39	6
ATOM	1258	C	GLY	988	25.704	30.203	-14.592	1.00 32.39	6
ATOM	1259	O	GLY	988	24.832	29.393	-14.275	1.00 32.39	8
ATOM	1260	N	GLN	989	26.999	29.978	-14.382	1.00 53.32	7
ATOM	1261	CA	GLN	989	27.473	28.756	-13.738	1.00 53.32	6
ATOM	1262	CB	GLN	989	28.063	27.789	-14.761	1.00 52.63	6
ATOM	1263	CG	GLN	989	27.056	26.759	-15.207	1.00 52.63	6
ATOM	1264	CD	GLN	989	27.583	25.337	-15.120	1.00 52.63	6
ATOM	1265	OE1	GLN	989	28.219	24.855	-16.052	1.00 52.63	8
ATOM	1266	NE2	GLN	989	27.355	24.672	-13.985	1.00 52.63	7
ATOM	1267	C	GLN	989	28.473	28.926	-12.631	1.00 53.32	6
ATOM	1268	O	GLN	989	28.683	28.002	-11.861	1.00 53.32	8
ATOM	1269	N	GLU	990	29.082	30.096	-12.532	1.00 57.00	7
ATOM	1270	CA	GLU	990	30.072	30.328	-11.503	1.00 57.00	6
ATOM	1271	CB	GLU	990	31.320	29.532	-11.858	1.00 60.46	6
ATOM	1272	CG	GLU	990	32.281	29.295	-10.745	1.00 60.46	6
ATOM	1273	CD	GLU	990	32.976	27.979	-10.927	1.00 60.46	6
ATOM	1274	OE1	GLU	990	33.448	27.718	-12.049	1.00 60.46	8
ATOM	1275	OE2	GLU	990	33.044	27.198	-9.960	1.00 60.46	8
ATOM	1276	C	GLU	990	30.368	31.814	-11.523	1.00 57.00	6
ATOM	1277	O	GLU	990	30.639	32.363	-12.589	1.00 57.00	8
ATOM	1278	N	VAL	991	30.269	32.470	-10.367	1.00 47.34	7
ATOM	1279	CA	VAL	991	30.567	33.904	-10.285	1.00 47.34	6
ATOM	1280	CB	VAL	991	29.423	34.745	-9.575	1.00 25.98	6
ATOM	1281	CG1	VAL	991	29.646	36.247	-9.822	1.00 25.98	6
ATOM	1282	CG2	VAL	991	28.029	34.365	-10.094	1.00 25.98	6
ATOM	1283	C	VAL	991	31.878	34.057	-9.493	1.00 47.34	6
ATOM	1284	O	VAL	991	32.387	33.090	-8.924	1.00 47.34	8
ATOM	1285	N	TYR	992	32.437	35.262	-9.483	1.00 68.84	7
ATOM	1286	CA	TYR	992	33.683	35.517	-8.774	1.00 68.84	6
ATOM	1287	CB	TYR	992	34.849	35.554	-9.765	1.00 49.61	6
ATOM	1288	CG	TYR	992	36.187	35.817	-9.103	1.00 49.61	6
ATOM	1289	CD1	TYR	992	36.680	34.950	-8.127	1.00 49.61	6
ATOM	1290	CE1	TYR	992	37.886	35.201	-7.465	1.00 49.61	6
ATOM	1291	CD2	TYR	992	36.941	36.947	-9.410	1.00 49.61	6
ATOM	1292	CE2	TYR	992	38.154	37.210	-8.750	1.00 49.61	6
ATOM	1293	CZ	TYR	992	38.614	36.333	-7.780	1.00 49.61	6
ATOM	1294	OH	TYR	992	39.785	36.607	-7.115	1.00 49.61	8
ATOM	1295	C	TYR	992	33.653	36.836	-7.999	1.00 68.84	6
ATOM	1296	O	TYR	992	33.941	37.886	-8.565	1.00 68.84	8
ATOM	1297	N	VAL	993	33.312	36.802	-6.718	1.00 73.45	7
ATOM	1298	CA	VAL	993	33.293	38.048	-5.964	1.00 73.45	6
ATOM	1299	CB	VAL	993	32.078	38.110	-5.043	1.00 77.88	6
ATOM	1300	CG1	VAL	993	30.812	38.281	-5.857	1.00 77.88	6

FIG. 3W

```
ATOM   1301  CG2 VAL   993      32.012  36.866  -4.236  1.00 77.88    6
ATOM   1302  C   VAL   993      34.585  38.227  -5.162  1.00 73.45    6
ATOM   1303  O   VAL   993      35.222  37.248  -4.762  1.00 73.45    8
ATOM   1304  N   LYS   994      34.965  39.483  -4.946  1.00100.00    7
ATOM   1305  CA  LYS   994      36.190  39.825  -4.225  1.00100.00    6
ATOM   1306  CB  LYS   994      37.340  39.934  -5.227  1.00 96.49    6
ATOM   1307  CG  LYS   994      38.693  40.258  -4.635  1.00 96.49    6
ATOM   1308  CD  LYS   994      39.679  40.656  -5.728  1.00 96.49    6
ATOM   1309  CE  LYS   994      40.977  39.891  -5.576  1.00 96.49    6
ATOM   1310  NZ  LYS   994      41.937  40.208  -6.655  1.00 96.49    7
ATOM   1311  C   LYS   994      35.981  41.170  -3.525  1.00100.00    6
ATOM   1312  O   LYS   994      36.298  42.217  -4.089  1.00100.00    8
ATOM   1313  N   LYS   995      35.456  41.135  -2.299  1.00100.00    7
ATOM   1314  CA  LYS   995      35.173  42.337  -1.505  1.00100.00    6
ATOM   1315  CB  LYS   995      36.432  43.233  -1.423  1.00100.00    6
ATOM   1316  C   LYS   995      33.996  43.132  -2.094  1.00100.00    6
ATOM   1317  O   LYS   995      34.079  44.383  -2.139  1.00100.00    8
ATOM   1318  OXT LYS   995      33.001  42.485  -2.484  1.00 85.30    8
TER
ATOM   1319  CB  PRO  1001      26.968  35.804   4.979  1.00 23.69    6
ATOM   1320  CG  PRO  1001      26.527  36.525   3.738  1.00 23.69    6
ATOM   1321  C   PRO  1001      29.219  34.895   5.215  1.00 43.97    6
ATOM   1322  O   PRO  1001      28.910  33.885   4.598  1.00 43.97    8
ATOM   1323  N   PRO  1001      28.835  36.609   3.692  1.00 43.97    7
ATOM   1324  CD  PRO  1001      27.692  36.488   2.779  1.00 23.69    6
ATOM   1325  CA  PRO  1001      28.434  36.157   5.028  1.00 43.97    6
ATOM   1326  N   VAL  1002      30.217  34.937   6.077  1.00 30.46    7
ATOM   1327  CA  VAL  1002      31.040  33.763   6.267  1.00 30.46    6
ATOM   1328  CB  VAL  1002      32.241  34.137   7.118  1.00 49.80    6
ATOM   1329  CG1 VAL  1002      32.805  35.456   6.632  1.00 49.80    6
ATOM   1330  CG2 VAL  1002      31.852  34.219   8.578  1.00 49.80    6
ATOM   1331  C   VAL  1002      30.360  32.503   6.834  1.00 30.46    6
ATOM   1332  O   VAL  1002      30.790  31.389   6.553  1.00 30.46    8
ATOM   1333  N   ARG  1003      29.292  32.669   7.596  1.00 40.35    7
ATOM   1334  CA  ARG  1003      28.643  31.505   8.207  1.00 40.35    6
ATOM   1335  CB  ARG  1003      27.872  31.924   9.444  1.00 42.33    6
ATOM   1336  CG  ARG  1003      28.755  32.265  10.626  1.00 42.33    6
ATOM   1337  CD  ARG  1003      27.857  32.633  11.767  1.00 42.33    6
ATOM   1338  NE  ARG  1003      28.533  32.694  13.047  1.00 42.33    7
ATOM   1339  CZ  ARG  1003      29.508  33.544  13.336  1.00 42.33    6
ATOM   1340  NH1 ARG  1003      29.932  34.417  12.428  1.00 42.33    7
ATOM   1341  NH2 ARG  1003      30.067  33.516  14.535  1.00 42.33    7
ATOM   1342  C   ARG  1003      27.737  30.626   7.370  1.00 40.35    6
ATOM   1343  O   ARG  1003      27.262  29.606   7.865  1.00 40.35    8
ATOM   1344  N   TRP  1004      27.495  31.011   6.121  1.00 26.04    7
ATOM   1345  CA  TRP  1004      26.632  30.250   5.221  1.00 26.04    6
ATOM   1346  CB  TRP  1004      25.459  31.141   4.768  1.00 50.68    6
ATOM   1347  CG  TRP  1004      24.332  31.279   5.776  1.00 50.68    6
ATOM   1348  CD2 TRP  1004      24.261  32.186   6.885  1.00 50.68    6
ATOM   1349  CE2 TRP  1004      23.066  31.901   7.585  1.00 50.68    6
ATOM   1350  CE3 TRP  1004      25.093  33.208   7.363  1.00 50.68    6
ATOM   1351  CD1 TRP  1004      23.207  30.513   5.843  1.00 50.68    6
ATOM   1352  NE1 TRP  1004      22.445  30.880   6.924  1.00 50.68    7
ATOM   1353  CZ2 TRP  1004      22.681  32.601   8.737  1.00 50.68    6
ATOM   1354  CZ3 TRP  1004      24.704  33.905   8.515  1.00 50.68    6
ATOM   1355  CH2 TRP  1004      23.510  33.594   9.186  1.00 50.68    6
ATOM   1356  C   TRP  1004      27.409  29.747   4.006  1.00 26.04    6
```

FIG. 3X

ATOM	1357	O	TRP	1004	27.003	28.794	3.356	1.00	26.04	8
ATOM	1358	N	MET	1005	28.535	30.382	3.706	1.00	37.80	7
ATOM	1359	CA	MET	1005	29.329	30.009	2.543	1.00	37.80	6
ATOM	1360	CB	MET	1005	30.502	30.949	2.412	1.00	40.16	6
ATOM	1361	CG	MET	1005	30.063	32.299	1.973	1.00	40.16	6
ATOM	1362	SD	MET	1005	31.319	33.493	2.212	1.00	40.16	16
ATOM	1363	CE	MET	1005	32.621	32.780	1.246	1.00	40.16	6
ATOM	1364	C	MET	1005	29.827	28.584	2.473	1.00	37.80	6
ATOM	1365	O	MET	1005	30.268	28.011	3.465	1.00	37.80	8
ATOM	1366	N	ALA	1006	29.753	28.008	1.283	1.00	45.98	7
ATOM	1367	CA	ALA	1006	30.230	26.654	1.092	1.00	45.98	6
ATOM	1368	CB	ALA	1006	29.797	26.138	-0.284	1.00	10.86	6
ATOM	1369	C	ALA	1006	31.764	26.736	1.196	1.00	45.98	6
ATOM	1370	O	ALA	1006	32.322	27.830	1.151	1.00	45.98	8
ATOM	1371	N	ILE	1007	32.448	25.604	1.326	1.00	44.58	7
ATOM	1372	CA	ILE	1007	33.909	25.657	1.446	1.00	44.58	6
ATOM	1373	CB	ILE	1007	34.528	24.267	1.753	1.00	25.13	6
ATOM	1374	CG2	ILE	1007	34.415	23.969	3.224	1.00	25.13	6
ATOM	1375	CG1	ILE	1007	33.880	23.182	0.886	1.00	25.13	6
ATOM	1376	CD1	ILE	1007	34.418	23.123	-0.571	1.00	25.13	6
ATOM	1377	C	ILE	1007	34.619	26.244	0.234	1.00	44.58	6
ATOM	1378	O	ILE	1007	35.585	26.988	0.379	1.00	44.58	8
ATOM	1379	N	GLU	1008	34.137	25.915	-0.957	1.00	31.07	7
ATOM	1380	CA	GLU	1008	34.743	26.402	-2.188	1.00	31.07	6
ATOM	1381	CB	GLU	1008	34.089	25.710	-3.378	1.00	43.81	6
ATOM	1382	CG	GLU	1008	32.595	25.941	-3.415	1.00	43.81	6
ATOM	1383	CD	GLU	1008	31.795	24.661	-3.241	1.00	43.81	6
ATOM	1384	OE1	GLU	1008	31.967	23.953	-2.216	1.00	43.81	8
ATOM	1385	OE2	GLU	1008	30.965	24.377	-4.125	1.00	43.81	8
ATOM	1386	C	GLU	1008	34.578	27.914	-2.308	1.00	31.07	6
ATOM	1387	O	GLU	1008	35.377	28.583	-2.967	1.00	31.07	8
ATOM	1388	N	SER	1009	33.546	28.447	-1.660	1.00	30.15	7
ATOM	1389	CA	SER	1009	33.259	29.873	-1.711	1.00	30.15	6
ATOM	1390	CB	SER	1009	31.802	30.117	-1.366	1.00	23.09	6
ATOM	1391	OG	SER	1009	30.984	29.174	-2.034	1.00	23.09	8
ATOM	1392	C	SER	1009	34.150	30.622	-0.743	1.00	30.15	6
ATOM	1393	O	SER	1009	34.565	31.760	-0.995	1.00	30.15	8
ATOM	1394	N	LEU	1010	34.428	29.977	0.381	1.00	29.90	7
ATOM	1395	CA	LEU	1010	35.293	30.566	1.380	1.00	29.90	6
ATOM	1396	CB	LEU	1010	35.402	29.629	2.585	1.00	44.65	6
ATOM	1397	CG	LEU	1010	34.152	29.450	3.460	1.00	44.65	6
ATOM	1398	CD1	LEU	1010	34.435	28.420	4.534	1.00	44.65	6
ATOM	1399	CD2	LEU	1010	33.752	30.781	4.101	1.00	44.65	6
ATOM	1400	C	LEU	1010	36.663	30.771	0.726	1.00	29.90	6
ATOM	1401	O	LEU	1010	37.082	31.912	0.503	1.00	29.90	8
ATOM	1402	N	ASN	1011	37.327	29.661	0.397	1.00	34.23	7
ATOM	1403	CA	ASN	1011	38.652	29.638	-0.230	1.00	34.23	6
ATOM	1404	CB	ASN	1011	39.105	28.205	-0.511	1.00	32.72	6
ATOM	1405	CG	ASN	1011	38.990	27.287	0.679	1.00	32.72	6
ATOM	1406	OD1	ASN	1011	39.433	27.600	1.783	1.00	32.72	8
ATOM	1407	ND2	ASN	1011	38.404	26.117	0.450	1.00	32.72	7
ATOM	1408	C	ASN	1011	38.801	30.353	-1.560	1.00	34.23	6
ATOM	1409	O	ASN	1011	39.728	31.137	-1.748	1.00	34.23	8
ATOM	1410	N	TYR	1012	37.914	30.041	-2.494	1.00	35.06	7
ATOM	1411	CA	TYR	1012	38.018	30.611	-3.822	1.00	35.06	6
ATOM	1412	CB	TYR	1012	37.824	29.521	-4.845	1.00	40.77	6
ATOM	1413	CG	TYR	1012	38.705	28.358	-4.552	1.00	40.77	6

FIG. 3Y

ATOM	1414	CD1	TYR	1012	38.167	27.093	-4.400	1.00	40.77	6
ATOM	1415	CE1	TYR	1012	38.961	26.024	-4.105	1.00	40.77	6
ATOM	1416	CD2	TYR	1012	40.077	28.531	-4.397	1.00	40.77	6
ATOM	1417	CE2	TYR	1012	40.896	27.472	-4.098	1.00	40.77	6
ATOM	1418	CZ	TYR	1012	40.336	26.208	-3.957	1.00	40.77	6
ATOM	1419	OH	TYR	1012	41.152	25.119	-3.717	1.00	40.77	8
ATOM	1420	C	TYR	1012	37.161	31.787	-4.193	1.00	35.06	6
ATOM	1421	O	TYR	1012	37.443	32.440	-5.195	1.00	35.06	8
ATOM	1422	N	SER	1013	36.109	32.060	-3.433	1.00	42.36	7
ATOM	1423	CA	SER	1013	35.278	33.209	-3.746	1.00	42.36	6
ATOM	1424	CB	SER	1013	36.159	34.439	-3.983	1.00	39.37	6
ATOM	1425	OG	SER	1013	37.157	34.576	-2.983	1.00	39.37	8
ATOM	1426	C	SER	1013	34.433	32.973	-4.982	1.00	42.36	6
ATOM	1427	O	SER	1013	34.291	33.865	-5.807	1.00	42.36	8
ATOM	1428	N	VAL	1014	33.890	31.772	-5.121	1.00	22.55	7
ATOM	1429	CA	VAL	1014	33.045	31.467	-6.260	1.00	22.55	6
ATOM	1430	CB	VAL	1014	33.653	30.369	-7.143	1.00	31.51	6
ATOM	1431	CG1	VAL	1014	35.048	30.791	-7.599	1.00	31.51	6
ATOM	1432	CG2	VAL	1014	33.701	29.054	-6.383	1.00	31.51	6
ATOM	1433	C	VAL	1014	31.720	30.999	-5.712	1.00	22.55	6
ATOM	1434	O	VAL	1014	31.644	30.562	-4.577	1.00	22.55	8
ATOM	1435	N	TYR	1015	30.671	31.121	-6.507	1.00	26.01	7
ATOM	1436	CA	TYR	1015	29.338	30.712	-6.101	1.00	26.01	6
ATOM	1437	CB	TYR	1015	28.501	31.938	-5.753	1.00	41.40	6
ATOM	1438	CG	TYR	1015	29.116	32.782	-4.672	1.00	41.40	6
ATOM	1439	CD1	TYR	1015	30.233	33.560	-4.922	1.00	41.40	6
ATOM	1440	CE1	TYR	1015	30.854	34.235	-3.904	1.00	41.40	6
ATOM	1441	CD2	TYR	1015	28.638	32.709	-3.365	1.00	41.40	6
ATOM	1442	CE2	TYR	1015	29.257	33.388	-2.330	1.00	41.40	6
ATOM	1443	CZ	TYR	1015	30.361	34.139	-2.605	1.00	41.40	6
ATOM	1444	OH	TYR	1015	30.968	34.830	-1.588	1.00	41.40	8
ATOM	1445	C	TYR	1015	28.674	29.998	-7.252	1.00	26.01	6
ATOM	1446	O	TYR	1015	28.513	30.572	-8.324	1.00	26.01	8
ATOM	1447	N	THR	1016	28.311	28.741	-7.043	1.00	17.46	7
ATOM	1448	CA	THR	1016	27.610	27.971	-8.082	1.00	17.46	6
ATOM	1449	CB	THR	1016	28.317	26.625	-8.456	1.00	15.11	6
ATOM	1450	OG1	THR	1016	28.649	25.909	-7.262	1.00	15.11	8
ATOM	1451	CG2	THR	1016	29.540	26.855	-9.283	1.00	15.11	6
ATOM	1452	C	THR	1016	26.257	27.590	-7.487	1.00	17.46	6
ATOM	1453	O	THR	1016	25.919	28.038	-6.408	1.00	17.46	8
ATOM	1454	N	THR	1017	25.489	26.752	-8.171	1.00	10.55	7
ATOM	1455	CA	THR	1017	24.229	26.325	-7.585	1.00	10.55	6
ATOM	1456	CB	THR	1017	23.346	25.602	-8.600	1.00	29.18	6
ATOM	1457	OG1	THR	1017	22.913	26.533	-9.600	1.00	29.18	8
ATOM	1458	CG2	THR	1017	22.138	25.017	-7.906	1.00	29.18	6
ATOM	1459	C	THR	1017	24.563	25.381	-6.419	1.00	10.55	6
ATOM	1460	O	THR	1017	23.802	25.287	-5.466	1.00	10.55	8
ATOM	1461	N	ASN	1018	25.740	24.743	-6.500	1.00	41.35	7
ATOM	1462	CA	ASN	1018	26.266	23.772	-5.505	1.00	41.35	6
ATOM	1463	CB	ASN	1018	27.522	23.095	-6.033	1.00	49.00	6
ATOM	1464	CG	ASN	1018	27.234	22.010	-7.015	1.00	49.00	6
ATOM	1465	OD1	ASN	1018	28.100	21.630	-7.788	1.00	49.00	8
ATOM	1466	ND2	ASN	1018	26.025	21.477	-6.981	1.00	49.00	7
ATOM	1467	C	ASN	1018	26.646	24.371	-4.156	1.00	41.35	6
ATOM	1468	O	ASN	1018	26.773	23.647	-3.160	1.00	41.35	8
ATOM	1469	N	SER	1019	26.887	25.680	-4.148	1.00	46.21	7
ATOM	1470	CA	SER	1019	27.247	26.400	-2.935	1.00	46.21	6

FIG. 3Z

ATOM	1471	CB	SER	1019	28.179	27.570	-3.247	1.00	35.31	6
ATOM	1472	OG	SER	1019	27.517	28.561	-3.996	1.00	35.31	8
ATOM	1473	C	SER	1019	25.936	26.919	-2.392	1.00	46.21	6
ATOM	1474	O	SER	1019	25.835	27.281	-1.225	1.00	46.21	8
ATOM	1475	N	ASP	1020	24.929	26.965	-3.253	1.00	42.68	7
ATOM	1476	CA	ASP	1020	23.640	27.426	-2.808	1.00	42.68	6
ATOM	1477	CB	ASP	1020	22.826	28.008	-3.951	1.00	34.86	6
ATOM	1478	CG	ASP	1020	22.962	29.508	-4.032	1.00	34.86	6
ATOM	1479	OD1	ASP	1020	23.242	30.127	-2.972	1.00	34.86	8
ATOM	1480	OD2	ASP	1020	22.788	30.046	-5.149	1.00	34.86	8
ATOM	1481	C	ASP	1020	22.912	26.281	-2.171	1.00	42.68	6
ATOM	1482	O	ASP	1020	21.925	26.487	-1.480	1.00	42.68	8
ATOM	1483	N	VAL	1021	23.401	25.071	-2.398	1.00	33.68	7
ATOM	1484	CA	VAL	1021	22.751	23.944	-1.787	1.00	33.68	6
ATOM	1485	CB	VAL	1021	22.872	22.690	-2.628	1.00	9.47	6
ATOM	1486	CG1	VAL	1021	22.096	21.575	-1.962	1.00	9.47	6
ATOM	1487	CG2	VAL	1021	22.328	22.940	-4.008	1.00	9.47	6
ATOM	1488	C	VAL	1021	23.403	23.746	-0.444	1.00	33.68	6
ATOM	1489	O	VAL	1021	22.872	23.061	0.422	1.00	33.68	8
ATOM	1490	N	TRP	1022	24.565	24.355	-0.268	1.00	49.04	7
ATOM	1491	CA	TRP	1022	25.247	24.284	1.011	1.00	49.04	6
ATOM	1492	CB	TRP	1022	26.732	24.600	0.868	1.00	36.23	6
ATOM	1493	CG	TRP	1022	27.463	24.712	2.164	1.00	36.23	6
ATOM	1494	CD2	TRP	1022	28.575	23.920	2.583	1.00	36.23	6
ATOM	1495	CE2	TRP	1022	28.985	24.411	3.836	1.00	36.23	6
ATOM	1496	CE3	TRP	1022	29.269	22.843	2.019	1.00	36.23	6
ATOM	1497	CD1	TRP	1022	27.246	25.623	3.158	1.00	36.23	6
ATOM	1498	NE1	TRP	1022	28.155	25.452	4.165	1.00	36.23	7
ATOM	1499	CZ2	TRP	1022	30.061	23.862	4.532	1.00	36.23	6
ATOM	1500	CZ3	TRP	1022	30.338	22.300	2.710	1.00	36.23	6
ATOM	1501	CH2	TRP	1022	30.721	22.808	3.951	1.00	36.23	6
ATOM	1502	C	TRP	1022	24.558	25.391	1.777	1.00	49.04	6
ATOM	1503	O	TRP	1022	23.962	25.164	2.822	1.00	49.04	8
ATOM	1504	N	SER	1023	24.599	26.598	1.244	1.00	20.71	7
ATOM	1505	CA	SER	1023	23.946	27.666	1.954	1.00	20.71	6
ATOM	1506	CB	SER	1023	24.032	28.977	1.181	1.00	17.98	6
ATOM	1507	OG	SER	1023	25.377	29.363	1.081	1.00	17.98	8
ATOM	1508	C	SER	1023	22.516	27.305	2.265	1.00	20.71	6
ATOM	1509	O	SER	1023	22.009	27.705	3.298	1.00	20.71	8
ATOM	1510	N	TYR	1024	21.842	26.557	1.400	1.00	27.47	7
ATOM	1511	CA	TYR	1024	20.474	26.200	1.758	1.00	27.47	6
ATOM	1512	CB	TYR	1024	19.728	25.580	0.590	1.00	25.94	6
ATOM	1513	CG	TYR	1024	18.447	24.902	1.003	1.00	25.94	6
ATOM	1514	CD1	TYR	1024	17.222	25.512	0.847	1.00	25.94	6
ATOM	1515	CE1	TYR	1024	16.037	24.846	1.170	1.00	25.94	6
ATOM	1516	CD2	TYR	1024	18.465	23.611	1.506	1.00	25.94	6
ATOM	1517	CE2	TYR	1024	17.288	22.954	1.833	1.00	25.94	6
ATOM	1518	CZ	TYR	1024	16.089	23.579	1.656	1.00	25.94	6
ATOM	1519	OH	TYR	1024	14.949	22.909	1.953	1.00	25.94	8
ATOM	1520	C	TYR	1024	20.502	25.233	2.942	1.00	27.47	6
ATOM	1521	O	TYR	1024	19.712	25.368	3.873	1.00	27.47	8
ATOM	1522	N	GLY	1025	21.419	24.273	2.917	1.00	24.43	7
ATOM	1523	CA	GLY	1025	21.505	23.344	4.025	1.00	24.43	6
ATOM	1524	C	GLY	1025	21.593	24.073	5.356	1.00	24.43	6
ATOM	1525	O	GLY	1025	21.032	23.619	6.356	1.00	24.43	8
ATOM	1526	N	VAL	1026	22.307	25.195	5.384	1.00	31.88	7
ATOM	1527	CA	VAL	1026	22.417	25.947	6.632	1.00	31.88	6

FIG. 3AA

ATOM	1528	CB	VAL	1026	23.566	26.979	6.609	1.00	14.56	6
ATOM	1529	CG1	VAL	1026	23.783	27.551	8.015	1.00	14.56	6
ATOM	1530	CG2	VAL	1026	24.835	26.301	6.132	1.00	14.56	6
ATOM	1531	C	VAL	1026	21.077	26.636	6.908	1.00	31.88	6
ATOM	1532	O	VAL	1026	20.691	26.833	8.062	1.00	31.88	8
ATOM	1533	N	LEU	1027	20.348	26.978	5.855	1.00	36.84	7
ATOM	1534	CA	LEU	1027	19.063	27.591	6.078	1.00	36.84	6
ATOM	1535	CB	LEU	1027	18.470	28.110	4.777	1.00	5.00	6
ATOM	1536	CG	LEU	1027	17.030	28.620	4.806	1.00	5.00	6
ATOM	1537	CD1	LEU	1027	16.683	29.318	6.095	1.00	5.00	6
ATOM	1538	CD2	LEU	1027	16.893	29.549	3.640	1.00	5.00	6
ATOM	1539	C	LEU	1027	18.149	26.556	6.711	1.00	36.84	6
ATOM	1540	O	LEU	1027	17.383	26.885	7.606	1.00	36.84	8
ATOM	1541	N	LEU	1028	18.234	25.304	6.272	1.00	19.77	7
ATOM	1542	CA	LEU	1028	17.390	24.264	6.848	1.00	19.77	6
ATOM	1543	CB	LEU	1028	17.645	22.931	6.147	1.00	24.80	6
ATOM	1544	CG	LEU	1028	16.802	21.696	6.487	1.00	24.80	6
ATOM	1545	CD1	LEU	1028	15.298	21.976	6.507	1.00	24.80	6
ATOM	1546	CD2	LEU	1028	17.117	20.681	5.417	1.00	24.80	6
ATOM	1547	C	LEU	1028	17.681	24.145	8.339	1.00	19.77	6
ATOM	1548	O	LEU	1028	16.779	23.912	9.136	1.00	19.77	8
ATOM	1549	N	TRP	1029	18.944	24.309	8.714	1.00	26.73	7
ATOM	1550	CA	TRP	1029	19.318	24.241	10.114	1.00	26.73	6
ATOM	1551	CB	TRP	1029	20.836	24.229	10.257	1.00	36.84	6
ATOM	1552	CG	TRP	1029	21.363	24.082	11.678	1.00	36.84	6
ATOM	1553	CD2	TRP	1029	21.634	25.145	12.611	1.00	36.84	6
ATOM	1554	CE2	TRP	1029	22.215	24.556	13.757	1.00	36.84	6
ATOM	1555	CE3	TRP	1029	21.438	26.536	12.588	1.00	36.84	6
ATOM	1556	CD1	TRP	1029	21.774	22.926	12.292	1.00	36.84	6
ATOM	1557	NE1	TRP	1029	22.292	23.202	13.539	1.00	36.84	7
ATOM	1558	CZ2	TRP	1029	22.613	25.310	14.860	1.00	36.84	6
ATOM	1559	CZ3	TRP	1029	21.830	27.283	13.682	1.00	36.84	6
ATOM	1560	CH2	TRP	1029	22.409	26.670	14.803	1.00	36.84	6
ATOM	1561	C	TRP	1029	18.736	25.435	10.898	1.00	26.73	6
ATOM	1562	O	TRP	1029	18.498	25.314	12.089	1.00	26.73	8
ATOM	1563	N	GLU	1030	18.520	26.590	10.266	1.00	28.62	7
ATOM	1564	CA	GLU	1030	17.958	27.734	10.996	1.00	28.62	6
ATOM	1565	CB	GLU	1030	18.082	29.020	10.177	1.00	33.13	6
ATOM	1566	CG	GLU	1030	19.486	29.535	10.077	1.00	33.13	6
ATOM	1567	CD	GLU	1030	19.635	30.718	9.135	1.00	33.13	6
ATOM	1568	OE1	GLU	1030	19.628	30.498	7.909	1.00	33.13	8
ATOM	1569	OE2	GLU	1030	19.756	31.865	9.625	1.00	33.13	8
ATOM	1570	C	GLU	1030	16.494	27.467	11.333	1.00	28.62	6
ATOM	1571	O	GLU	1030	16.066	27.619	12.470	1.00	28.62	8
ATOM	1572	N	ILE	1031	15.746	27.065	10.314	1.00	23.86	7
ATOM	1573	CA	ILE	1031	14.328	26.733	10.413	1.00	23.86	6
ATOM	1574	CB	ILE	1031	13.845	26.094	9.083	1.00	5.00	6
ATOM	1575	CG2	ILE	1031	12.626	25.263	9.308	1.00	5.00	6
ATOM	1576	CG1	ILE	1031	13.660	27.181	8.029	1.00	5.00	6
ATOM	1577	CD1	ILE	1031	13.157	26.703	6.709	1.00	5.00	6
ATOM	1578	C	ILE	1031	14.085	25.760	11.544	1.00	23.86	6
ATOM	1579	O	ILE	1031	13.202	25.946	12.357	1.00	23.86	8
ATOM	1580	N	VAL	1032	14.894	24.723	11.595	1.00	16.66	7
ATOM	1581	CA	VAL	1032	14.745	23.717	12.611	1.00	16.66	6
ATOM	1582	CB	VAL	1032	15.538	22.452	12.184	1.00	12.88	6
ATOM	1583	CG1	VAL	1032	15.873	21.594	13.367	1.00	12.88	6
ATOM	1584	CG2	VAL	1032	14.713	21.662	11.163	1.00	12.88	6

FIG. 3BB

ATOM	1585	C	VAL	1032	15.155	24.252	13.977	1.00	16.66	6
ATOM	1586	O	VAL	1032	14.456	24.032	14.952	1.00	16.66	8
ATOM	1587	N	SER	1033	16.258	24.986	14.058	1.00	33.94	7
ATOM	1588	CA	SER	1033	16.732	25.551	15.331	1.00	33.94	6
ATOM	1589	CB	SER	1033	18.173	25.982	15.197	1.00	27.55	6
ATOM	1590	OG	SER	1033	18.203	27.172	14.452	1.00	27.55	8
ATOM	1591	C	SER	1033	15.937	26.791	15.793	1.00	33.94	6
ATOM	1592	O	SER	1033	16.275	27.415	16.801	1.00	33.94	8
ATOM	1593	N	LEU	1034	14.913	27.165	15.035	1.00	25.63	7
ATOM	1594	CA	LEU	1034	14.075	28.313	15.353	1.00	25.63	6
ATOM	1595	CB	LEU	1034	13.382	28.107	16.707	1.00	16.09	6
ATOM	1596	CG	LEU	1034	12.545	26.834	16.882	1.00	16.09	6
ATOM	1597	CD1	LEU	1034	11.931	26.831	18.286	1.00	16.09	6
ATOM	1598	CD2	LEU	1034	11.456	26.758	15.839	1.00	16.09	6
ATOM	1599	C	LEU	1034	14.777	29.676	15.328	1.00	25.63	6
ATOM	1600	O	LEU	1034	14.641	30.476	16.254	1.00	25.63	8
ATOM	1601	N	GLY	1035	15.519	29.927	14.256	1.00	32.06	7
ATOM	1602	CA	GLY	1035	16.185	31.202	14.092	1.00	32.06	6
ATOM	1603	C	GLY	1035	17.458	31.404	14.866	1.00	32.06	6
ATOM	1604	O	GLY	1035	17.832	32.537	15.149	1.00	32.06	8
ATOM	1605	N	GLY	1036	18.124	30.316	15.224	1.00	12.96	7
ATOM	1606	CA	GLY	1036	19.371	30.430	15.957	1.00	12.96	6
ATOM	1607	C	GLY	1036	20.486	30.704	14.974	1.00	12.96	6
ATOM	1608	O	GLY	1036	20.355	30.393	13.789	1.00	12.96	8
ATOM	1609	N	THR	1037	21.572	31.293	15.457	1.00	38.43	7
ATOM	1610	CA	THR	1037	22.712	31.608	14.609	1.00	38.43	6
ATOM	1611	CB	THR	1037	23.593	32.723	15.266	1.00	32.45	6
ATOM	1612	OG1	THR	1037	22.813	33.907	15.442	1.00	32.45	8
ATOM	1613	CG2	THR	1037	24.754	33.076	14.387	1.00	32.45	6
ATOM	1614	C	THR	1037	23.519	30.323	14.418	1.00	38.43	6
ATOM	1615	O	THR	1037	23.687	29.555	15.359	1.00	38.43	8
ATOM	1616	N	PRO	1038	24.003	30.054	13.193	1.00	51.13	7
ATOM	1617	CD	PRO	1038	23.734	30.837	11.973	1.00	42.78	6
ATOM	1618	CA	PRO	1038	24.791	28.859	12.863	1.00	51.13	6
ATOM	1619	CB	PRO	1038	24.677	28.776	11.354	1.00	42.78	6
ATOM	1620	CG	PRO	1038	24.691	30.218	10.977	1.00	42.78	6
ATOM	1621	C	PRO	1038	26.233	28.968	13.308	1.00	51.13	6
ATOM	1622	O	PRO	1038	26.873	30.002	13.113	1.00	51.13	8
ATOM	1623	N	TYR	1039	26.753	27.895	13.886	1.00	44.91	7
ATOM	1624	CA	TYR	1039	28.124	27.909	14.349	1.00	44.91	6
ATOM	1625	CB	TYR	1039	29.082	28.341	13.221	1.00	38.97	6
ATOM	1626	CG	TYR	1039	28.980	27.544	11.933	1.00	38.97	6
ATOM	1627	CD1	TYR	1039	28.593	28.161	10.739	1.00	38.97	6
ATOM	1628	CE1	TYR	1039	28.487	27.434	9.545	1.00	38.97	6
ATOM	1629	CD2	TYR	1039	29.263	26.185	11.907	1.00	38.97	6
ATOM	1630	CE2	TYR	1039	29.165	25.455	10.730	1.00	38.97	6
ATOM	1631	CZ	TYR	1039	28.773	26.082	9.553	1.00	38.97	6
ATOM	1632	OH	TYR	1039	28.647	25.353	8.396	1.00	38.97	8
ATOM	1633	C	TYR	1039	28.176	28.932	15.479	1.00	44.91	6
ATOM	1634	O	TYR	1039	29.152	29.674	15.601	1.00	44.91	8
ATOM	1635	N	CYS	1040	27.120	28.989	16.293	1.00	52.33	7
ATOM	1636	CA	CYS	1040	27.093	29.933	17.411	1.00	52.33	6
ATOM	1637	CB	CYS	1040	25.700	30.015	18.046	1.00	51.31	6
ATOM	1638	SG	CYS	1040	25.484	31.409	19.213	1.00	51.31	16
ATOM	1639	C	CYS	1040	28.094	29.416	18.424	1.00	52.33	6
ATOM	1640	O	CYS	1040	28.113	28.224	18.729	1.00	52.33	8
ATOM	1641	N	GLY	1041	28.930	30.315	18.928	1.00	33.04	7

FIG. 3CC

ATOM	1642	CA	GLY	1041	29.930	29.917	19.895	1.00	33.04	6
ATOM	1643	C	GLY	1041	31.293	29.745	19.257	1.00	33.04	6
ATOM	1644	O	GLY	1041	32.207	29.176	19.855	1.00	33.04	8
ATOM	1645	N	MET	1042	31.435	30.206	18.024	1.00	54.51	7
ATOM	1646	CA	MET	1042	32.718	30.129	17.350	1.00	54.51	6
ATOM	1647	CB	MET	1042	32.703	29.085	16.241	1.00	40.53	6
ATOM	1648	CG	MET	1042	33.032	27.691	16.710	1.00	40.53	6
ATOM	1649	SD	MET	1042	32.920	26.501	15.349	1.00	40.53	16
ATOM	1650	CE	MET	1042	31.539	25.362	15.966	1.00	40.53	6
ATOM	1651	C	MET	1042	33.029	31.492	16.785	1.00	54.51	6
ATOM	1652	O	MET	1042	32.195	32.395	16.804	1.00	54.51	8
ATOM	1653	N	THR	1043	34.241	31.633	16.286	1.00	54.86	7
ATOM	1654	CA	THR	1043	34.677	32.894	15.726	1.00	54.86	6
ATOM	1655	CB	THR	1043	36.055	33.252	16.229	1.00	82.76	6
ATOM	1656	OG1	THR	1043	36.987	32.269	15.763	1.00	82.76	8
ATOM	1657	CG2	THR	1043	36.069	33.282	17.735	1.00	82.76	6
ATOM	1658	C	THR	1043	34.780	32.796	14.227	1.00	54.86	6
ATOM	1659	O	THR	1043	34.695	31.710	13.659	1.00	54.86	8
ATOM	1660	N	CYS	1044	35.002	33.943	13.599	1.00	95.17	7
ATOM	1661	CA	CYS	1044	35.142	34.000	12.158	1.00	95.17	6
ATOM	1662	CB	CYS	1044	35.205	35.453	11.692	1.00	93.17	6
ATOM	1663	SG	CYS	1044	33.676	36.379	11.856	1.00	93.17	16
ATOM	1664	C	CYS	1044	36.396	33.272	11.681	1.00	95.17	6
ATOM	1665	O	CYS	1044	36.622	33.174	10.483	1.00	95.17	8
ATOM	1666	N	ALA	1045	37.215	32.773	12.603	1.00	38.28	7
ATOM	1667	CA	ALA	1045	38.428	32.079	12.197	1.00	38.28	6
ATOM	1668	CB	ALA	1045	39.618	32.633	12.941	1.00	50.33	6
ATOM	1669	C	ALA	1045	38.348	30.571	12.387	1.00	38.28	6
ATOM	1670	O	ALA	1045	38.780	29.817	11.517	1.00	38.28	8
ATOM	1671	N	GLU	1046	37.822	30.131	13.526	1.00	39.84	7
ATOM	1672	CA	GLU	1046	37.712	28.702	13.787	1.00	39.84	6
ATOM	1673	CB	GLU	1046	36.911	28.460	15.068	1.00	83.44	6
ATOM	1674	CG	GLU	1046	37.622	28.995	16.300	1.00	83.44	6
ATOM	1675	CD	GLU	1046	36.997	28.556	17.607	1.00	83.44	6
ATOM	1676	OE1	GLU	1046	36.872	27.334	17.835	1.00	83.44	8
ATOM	1677	OE2	GLU	1046	36.635	29.442	18.408	1.00	83.44	8
ATOM	1678	C	GLU	1046	37.051	28.027	12.591	1.00	39.84	6
ATOM	1679	O	GLU	1046	37.370	26.884	12.245	1.00	39.84	8
ATOM	1680	N	LEU	1047	36.148	28.772	11.953	1.00	55.18	7
ATOM	1681	CA	LEU	1047	35.412	28.312	10.771	1.00	55.18	6
ATOM	1682	CB	LEU	1047	34.315	29.319	10.424	1.00	58.88	6
ATOM	1683	CG	LEU	1047	33.325	29.563	11.565	1.00	58.88	6
ATOM	1684	CD1	LEU	1047	32.333	30.619	11.148	1.00	58.88	6
ATOM	1685	CD2	LEU	1047	32.610	28.260	11.906	1.00	58.88	6
ATOM	1686	C	LEU	1047	36.307	28.092	9.548	1.00	55.18	6
ATOM	1687	O	LEU	1047	36.106	27.157	8.786	1.00	55.18	8
ATOM	1688	N	TYR	1048	37.283	28.967	9.352	1.00	49.08	7
ATOM	1689	CA	TYR	1048	38.203	28.820	8.234	1.00	49.08	6
ATOM	1690	CB	TYR	1048	39.033	30.097	8.078	1.00	62.53	6
ATOM	1691	CG	TYR	1048	38.422	31.088	7.123	1.00	62.53	6
ATOM	1692	CD1	TYR	1048	37.554	32.092	7.559	1.00	62.53	6
ATOM	1693	CE1	TYR	1048	36.956	32.963	6.644	1.00	62.53	6
ATOM	1694	CD2	TYR	1048	38.678	30.981	5.765	1.00	62.53	6
ATOM	1695	CE2	TYR	1048	38.096	31.829	4.851	1.00	62.53	6
ATOM	1696	CZ	TYR	1048	37.233	32.820	5.280	1.00	62.53	6
ATOM	1697	OH	TYR	1048	36.649	33.642	4.333	1.00	62.53	8
ATOM	1698	C	TYR	1048	39.112	27.618	8.525	1.00	49.08	6

FIG. 3DD

ATOM	1699	O	TYR	1048	39.661	27.008	7.603	1.00 49.08	8
ATOM	1700	N	GLU	1049	39.224	27.293	9.817	1.00 50.97	7
ATOM	1701	CA	GLU	1049	40.047	26.196	10.341	1.00 50.97	6
ATOM	1702	CB	GLU	1049	40.532	26.543	11.761	1.00 95.40	6
ATOM	1703	CG	GLU	1049	41.455	25.483	12.408	1.00 95.40	6
ATOM	1704	CD	GLU	1049	41.583	25.610	13.940	1.00 95.40	6
ATOM	1705	OE1	GLU	1049	41.872	26.717	14.445	1.00 95.40	8
ATOM	1706	OE2	GLU	1049	41.397	24.589	14.641	1.00 95.40	8
ATOM	1707	C	GLU	1049	39.347	24.829	10.395	1.00 50.97	6
ATOM	1708	O	GLU	1049	39.581	23.962	9.543	1.00 50.97	8
ATOM	1709	N	LYS	1050	38.499	24.659	11.416	1.00 80.24	7
ATOM	1710	CA	LYS	1050	37.750	23.420	11.683	1.00 80.24	6
ATOM	1711	CB	LYS	1050	37.217	23.446	13.105	1.00 32.58	6
ATOM	1712	C	LYS	1050	36.603	23.121	10.729	1.00 80.24	6
ATOM	1713	O	LYS	1050	35.910	22.112	10.874	1.00 80.24	8
ATOM	1714	N	LEU	1051	36.394	23.993	9.757	1.00 50.22	7
ATOM	1715	CA	LEU	1051	35.323	23.769	8.810	1.00 50.22	6
ATOM	1716	CB	LEU	1051	34.627	25.081	8.449	1.00 21.77	6
ATOM	1717	CG	LEU	1051	33.258	24.954	7.780	1.00 21.77	6
ATOM	1718	CD1	LEU	1051	32.248	24.632	8.834	1.00 21.77	6
ATOM	1719	CD2	LEU	1051	32.900	26.226	7.065	1.00 21.77	6
ATOM	1720	C	LEU	1051	35.827	23.121	7.540	1.00 50.22	6
ATOM	1721	O	LEU	1051	35.308	22.098	7.123	1.00 50.22	8
ATOM	1722	N	PRO	1052	36.860	23.692	6.913	1.00 73.14	7
ATOM	1723	CD	PRO	1052	37.819	24.695	7.400	1.00 57.36	6
ATOM	1724	CA	PRO	1052	37.372	23.122	5.675	1.00 73.14	6
ATOM	1725	CB	PRO	1052	38.669	23.898	5.460	1.00 57.36	6
ATOM	1726	CG	PRO	1052	38.368	25.214	6.097	1.00 57.36	6
ATOM	1727	C	PRO	1052	37.600	21.638	5.814	1.00 73.14	6
ATOM	1728	O	PRO	1052	36.747	20.823	5.474	1.00 73.14	8
ATOM	1729	N	GLN	1053	38.756	21.308	6.359	1.00 77.10	7
ATOM	1730	CA	GLN	1053	39.139	19.932	6.542	1.00 77.10	6
ATOM	1731	CB	GLN	1053	40.574	19.886	7.003	1.00100.00	6
ATOM	1732	C	GLN	1053	38.256	19.137	7.504	1.00 77.10	6
ATOM	1733	O	GLN	1053	38.279	17.904	7.479	1.00 77.10	8
ATOM	1734	N	GLY	1054	37.475	19.815	8.341	1.00 78.88	7
ATOM	1735	CA	GLY	1054	36.658	19.075	9.293	1.00 78.88	6
ATOM	1736	C	GLY	1054	35.160	18.960	9.074	1.00 78.88	6
ATOM	1737	O	GLY	1054	34.644	19.099	7.965	1.00 78.88	8
ATOM	1738	N	TYR	1055	34.460	18.683	10.164	1.00 61.80	7
ATOM	1739	CA	TYR	1055	33.018	18.525	10.146	1.00 61.80	6
ATOM	1740	CB	TYR	1055	32.547	17.902	11.458	1.00100.00	6
ATOM	1741	CG	TYR	1055	32.642	18.897	12.598	1.00100.00	6
ATOM	1742	CD1	TYR	1055	31.499	19.464	13.161	1.00100.00	6
ATOM	1743	CE1	TYR	1055	31.592	20.444	14.144	1.00100.00	6
ATOM	1744	CD2	TYR	1055	33.885	19.337	13.057	1.00100.00	6
ATOM	1745	CE2	TYR	1055	33.985	20.316	14.039	1.00100.00	6
ATOM	1746	CZ	TYR	1055	32.835	20.860	14.571	1.00100.00	6
ATOM	1747	OH	TYR	1055	32.928	21.827	15.531	1.00100.00	8
ATOM	1748	C	TYR	1055	32.344	19.891	10.001	1.00 61.80	6
ATOM	1749	O	TYR	1055	32.982	20.912	9.728	1.00 61.80	8
ATOM	1750	N	ARG	1056	31.038	19.885	10.231	1.00 78.80	7
ATOM	1751	CA	ARG	1056	30.216	21.079	10.155	1.00 78.80	6
ATOM	1752	CB	ARG	1056	29.674	21.216	8.729	1.00 56.27	6
ATOM	1753	CG	ARG	1056	29.456	19.890	8.001	1.00 56.27	6
ATOM	1754	CD	ARG	1056	29.992	19.943	6.563	1.00 56.27	6
ATOM	1755	NE	ARG	1056	31.444	19.832	6.494	1.00 56.27	7

FIG. 3EE

ATOM	1756	CZ	ARG	1056	32.115	19.413	5.425	1.00	56.27	6
ATOM	1757	NH1	ARG	1056	31.468	19.062	4.323	1.00	56.27	7
ATOM	1758	NH2	ARG	1056	33.441	19.327	5.464	1.00	56.27	7
ATOM	1759	C	ARG	1056	29.074	21.074	11.192	1.00	78.80	6
ATOM	1760	O	ARG	1056	29.031	20.212	12.068	1.00	78.80	8
ATOM	1761	N	LEU	1057	28.149	22.030	11.081	1.00	52.45	7
ATOM	1762	CA	LEU	1057	27.019	22.181	12.016	1.00	52.45	6
ATOM	1763	CB	LEU	1057	25.915	23.018	11.375	1.00	37.29	6
ATOM	1764	CG	LEU	1057	26.218	24.496	11.647	1.00	37.29	6
ATOM	1765	CD1	LEU	1057	25.208	25.439	10.966	1.00	37.29	6
ATOM	1766	CD2	LEU	1057	26.201	24.676	13.134	1.00	37.29	6
ATOM	1767	C	LEU	1057	26.429	20.921	12.635	1.00	52.45	6
ATOM	1768	O	LEU	1057	26.147	19.948	11.957	1.00	52.45	8
ATOM	1769	N	GLU	1058	26.264	20.978	13.955	1.00	65.26	7
ATOM	1770	CA	GLU	1058	25.730	19.856	14.739	1.00	65.26	6
ATOM	1771	CB	GLU	1058	26.251	19.940	16.182	1.00	73.19	6
ATOM	1772	CG	GLU	1058	25.940	21.232	16.943	1.00	73.19	6
ATOM	1773	CD	GLU	1058	26.617	22.490	16.375	1.00	73.19	6
ATOM	1774	OE1	GLU	1058	27.625	22.354	15.641	1.00	73.19	8
ATOM	1775	OE2	GLU	1058	26.158	23.611	16.679	1.00	73.19	8
ATOM	1776	C	GLU	1058	24.207	19.746	14.738	1.00	65.26	6
ATOM	1777	O	GLU	1058	23.497	20.746	14.708	1.00	65.26	8
ATOM	1778	N	LYS	1059	23.721	18.509	14.777	1.00	77.52	7
ATOM	1779	CA	LYS	1059	22.282	18.230	14.756	1.00	77.52	6
ATOM	1780	CB	LYS	1059	22.021	16.720	14.580	1.00	63.67	6
ATOM	1781	CG	LYS	1059	20.563	16.341	14.799	1.00	63.67	6
ATOM	1782	CD	LYS	1059	20.206	15.034	14.104	1.00	63.67	6
ATOM	1783	CE	LYS	1059	20.288	13.847	15.043	1.00	63.67	6
ATOM	1784	NZ	LYS	1059	19.240	13.976	16.098	1.00	63.67	7
ATOM	1785	C	LYS	1059	21.507	18.697	15.978	1.00	77.52	6
ATOM	1786	O	LYS	1059	21.765	18.261	17.093	1.00	77.52	8
ATOM	1787	N	PRO	1060	20.530	19.587	15.780	1.00	65.64	7
ATOM	1788	CD	PRO	1060	20.131	20.220	14.513	1.00	37.22	6
ATOM	1789	CA	PRO	1060	19.725	20.087	16.894	1.00	65.64	6
ATOM	1790	CB	PRO	1060	18.724	21.016	16.219	1.00	37.22	6
ATOM	1791	CG	PRO	1060	19.416	21.473	14.984	1.00	37.22	6
ATOM	1792	C	PRO	1060	19.030	18.898	17.567	1.00	65.64	6
ATOM	1793	O	PRO	1060	18.860	17.840	16.956	1.00	65.64	8
ATOM	1794	N	LEU	1061	18.637	19.074	18.820	1.00	79.51	7
ATOM	1795	CA	LEU	1061	17.962	18.017	19.564	1.00	79.51	6
ATOM	1796	CB	LEU	1061	17.893	18.413	21.044	1.00	82.15	6
ATOM	1797	CG	LEU	1061	17.476	19.851	21.443	1.00	82.15	6
ATOM	1798	CD1	LEU	1061	18.413	20.859	20.777	1.00	82.15	6
ATOM	1799	CD2	LEU	1061	16.033	20.116	21.048	1.00	82.15	6
ATOM	1800	C	LEU	1061	16.562	17.680	19.047	1.00	79.51	6
ATOM	1801	O	LEU	1061	16.187	16.513	19.026	1.00	79.51	8
ATOM	1802	N	ASN	1062	15.802	18.696	18.631	1.00	43.98	7
ATOM	1803	CA	ASN	1062	14.437	18.512	18.124	1.00	43.98	6
ATOM	1804	CB	ASN	1062	13.689	19.843	18.124	1.00	26.42	6
ATOM	1805	CG	ASN	1062	14.462	20.938	17.404	1.00	26.42	6
ATOM	1806	OD1	ASN	1062	15.554	21.327	17.834	1.00	26.42	8
ATOM	1807	ND2	ASN	1062	13.908	21.430	16.294	1.00	26.42	7
ATOM	1808	C	ASN	1062	14.459	17.989	16.718	1.00	43.98	6
ATOM	1809	O	ASN	1062	13.422	17.665	16.156	1.00	43.98	8
ATOM	1810	N	CYS	1063	15.646	17.914	16.143	1.00	48.23	7
ATOM	1811	CA	CYS	1063	15.767	17.460	14.769	1.00	48.23	6
ATOM	1812	CB	CYS	1063	16.914	18.199	14.103	1.00	49.76	6

FIG. 3FF

ATOM	1813	SG	CYS	1063	16.932	17.981	12.363	1.00	49.76	16
ATOM	1814	C	CYS	1063	15.943	15.948	14.559	1.00	48.23	6
ATOM	1815	O	CYS	1063	16.912	15.361	15.039	1.00	48.23	8
ATOM	1816	N	ASP	1064	15.001	15.338	13.834	1.00	41.84	7
ATOM	1817	CA	ASP	1064	15.029	13.907	13.522	1.00	41.84	6
ATOM	1818	CB	ASP	1064	13.788	13.487	12.715	1.00	55.35	6
ATOM	1819	CG	ASP	1064	13.829	12.012	12.290	1.00	55.35	6
ATOM	1820	OD1	ASP	1064	13.977	11.154	13.175	1.00	55.35	8
ATOM	1821	OD2	ASP	1064	13.712	11.710	11.086	1.00	55.35	8
ATOM	1822	C	ASP	1064	16.273	13.599	12.702	1.00	41.84	6
ATOM	1823	O	ASP	1064	16.918	14.521	12.181	1.00	41.84	8
ATOM	1824	N	ASP	1065	16.602	12.309	12.576	1.00	68.56	7
ATOM	1825	CA	ASP	1065	17.789	11.871	11.825	1.00	68.56	6
ATOM	1826	CB	ASP	1065	18.094	10.391	12.086	1.00	100.00	6
ATOM	1827	CG	ASP	1065	18.357	10.088	13.549	1.00	100.00	6
ATOM	1828	OD1	ASP	1065	17.400	10.124	14.341	1.00	100.00	8
ATOM	1829	OD2	ASP	1065	19.524	9.820	13.894	1.00	100.00	8
ATOM	1830	C	ASP	1065	17.654	12.072	10.321	1.00	68.56	6
ATOM	1831	O	ASP	1065	18.627	12.404	9.644	1.00	68.56	8
ATOM	1832	N	GLU	1066	16.457	11.850	9.797	1.00	54.29	7
ATOM	1833	CA	GLU	1066	16.247	12.025	8.378	1.00	54.29	6
ATOM	1834	CB	GLU	1066	14.843	11.583	8.001	1.00	91.86	6
ATOM	1835	CG	GLU	1066	14.550	10.152	8.383	1.00	91.86	6
ATOM	1836	CD	GLU	1066	13.252	9.651	7.787	1.00	91.86	6
ATOM	1837	OE1	GLU	1066	12.729	8.615	8.258	1.00	91.86	8
ATOM	1838	OE2	GLU	1066	12.755	10.296	6.840	1.00	91.86	8
ATOM	1839	C	GLU	1066	16.481	13.479	7.989	1.00	54.29	6
ATOM	1840	O	GLU	1066	17.223	13.758	7.048	1.00	54.29	8
ATOM	1841	N	VAL	1067	15.878	14.408	8.727	1.00	46.62	7
ATOM	1842	CA	VAL	1067	16.032	15.836	8.426	1.00	46.62	6
ATOM	1843	CB	VAL	1067	15.277	16.712	9.430	1.00	20.69	6
ATOM	1844	CG1	VAL	1067	15.286	18.154	8.957	1.00	20.69	6
ATOM	1845	CG2	VAL	1067	13.879	16.208	9.595	1.00	20.69	6
ATOM	1846	C	VAL	1067	17.484	16.314	8.400	1.00	46.62	6
ATOM	1847	O	VAL	1067	17.892	17.076	7.526	1.00	46.62	8
ATOM	1848	N	TYR	1068	18.261	15.858	9.367	1.00	49.64	7
ATOM	1849	CA	TYR	1068	19.654	16.240	9.459	1.00	49.64	6
ATOM	1850	CB	TYR	1068	20.195	15.811	10.813	1.00	42.96	6
ATOM	1851	CG	TYR	1068	21.604	16.239	11.074	1.00	42.96	6
ATOM	1852	CD1	TYR	1068	21.947	17.594	11.093	1.00	42.96	6
ATOM	1853	CE1	TYR	1068	23.236	18.006	11.387	1.00	42.96	6
ATOM	1854	CD2	TYR	1068	22.593	15.301	11.348	1.00	42.96	6
ATOM	1855	CE2	TYR	1068	23.882	15.701	11.640	1.00	42.96	6
ATOM	1856	CZ	TYR	1068	24.198	17.055	11.662	1.00	42.96	6
ATOM	1857	OH	TYR	1068	25.470	17.451	11.985	1.00	42.96	8
ATOM	1858	C	TYR	1068	20.424	15.557	8.338	1.00	49.64	6
ATOM	1859	O	TYR	1068	21.239	16.176	7.663	1.00	49.64	8
ATOM	1860	N	ASP	1069	20.148	14.275	8.144	1.00	54.25	7
ATOM	1861	CA	ASP	1069	20.808	13.495	7.112	1.00	54.25	6
ATOM	1862	CB	ASP	1069	20.056	12.188	6.905	1.00	100.00	6
ATOM	1863	CG	ASP	1069	20.812	11.231	6.043	1.00	100.00	6
ATOM	1864	OD1	ASP	1069	21.225	11.635	4.937	1.00	100.00	8
ATOM	1865	OD2	ASP	1069	20.986	10.076	6.479	1.00	100.00	8
ATOM	1866	C	ASP	1069	20.815	14.279	5.803	1.00	54.25	6
ATOM	1867	O	ASP	1069	21.779	14.247	5.037	1.00	54.25	8
ATOM	1868	N	LEU	1070	19.697	14.956	5.562	1.00	40.31	7
ATOM	1869	CA	LEU	1070	19.496	15.777	4.371	1.00	40.31	6

FIG. 3GG

ATOM	1870	CB	LEU	1070	18.009	16.075	4.195	1.00	25.05	6
ATOM	1871	CG	LEU	1070	17.581	16.966	3.048	1.00	25.05	6
ATOM	1872	CD1	LEU	1070	17.865	16.291	1.720	1.00	25.05	6
ATOM	1873	CD2	LEU	1070	16.114	17.219	3.219	1.00	25.05	6
ATOM	1874	C	LEU	1070	20.290	17.079	4.447	1.00	40.31	6
ATOM	1875	O	LEU	1070	20.561	17.688	3.423	1.00	40.31	8
ATOM	1876	N	MET	1071	20.639	17.510	5.655	1.00	23.05	7
ATOM	1877	CA	MET	1071	21.452	18.703	5.785	1.00	23.05	6
ATOM	1878	CB	MET	1071	21.367	19.310	7.201	1.00	19.93	6
ATOM	1879	CG	MET	1071	20.030	19.910	7.631	1.00	19.93	6
ATOM	1880	SD	MET	1071	20.077	20.344	9.411	1.00	19.93	16
ATOM	1881	CE	MET	1071	18.390	20.649	9.751	1.00	19.93	6
ATOM	1882	C	MET	1071	22.888	18.243	5.504	1.00	23.05	6
ATOM	1883	O	MET	1071	23.591	18.880	4.744	1.00	23.05	8
ATOM	1884	N	ARG	1072	23.319	17.124	6.082	1.00	51.65	7
ATOM	1885	CA	ARG	1072	24.689	16.669	5.864	1.00	51.65	6
ATOM	1886	CB	ARG	1072	24.978	15.434	6.696	1.00	98.84	6
ATOM	1887	CG	ARG	1072	24.870	15.716	8.162	1.00	98.84	6
ATOM	1888	CD	ARG	1072	26.125	16.339	8.727	1.00	98.84	6
ATOM	1889	NE	ARG	1072	27.004	15.305	9.271	1.00	98.84	7
ATOM	1890	CZ	ARG	1072	27.992	15.530	10.131	1.00	98.84	6
ATOM	1891	NH1	ARG	1072	28.232	16.767	10.546	1.00	98.84	7
ATOM	1892	NH2	ARG	1072	28.724	14.521	10.593	1.00	98.84	7
ATOM	1893	C	ARG	1072	25.023	16.404	4.401	1.00	51.65	6
ATOM	1894	O	ARG	1072	26.150	16.659	3.973	1.00	51.65	8
ATOM	1895	N	GLN	1073	24.073	15.900	3.617	1.00	27.54	7
ATOM	1896	CA	GLN	1073	24.376	15.679	2.211	1.00	27.54	6
ATOM	1897	CB	GLN	1073	23.347	14.746	1.568	1.00	67.93	6
ATOM	1898	CG	GLN	1073	21.934	15.149	1.789	1.00	67.93	6
ATOM	1899	CD	GLN	1073	20.972	14.026	1.527	1.00	67.93	6
ATOM	1900	OE1	GLN	1073	20.889	13.066	2.298	1.00	67.93	8
ATOM	1901	NE2	GLN	1073	20.238	14.127	0.422	1.00	67.93	7
ATOM	1902	C	GLN	1073	24.449	17.041	1.500	1.00	27.54	6
ATOM	1903	O	GLN	1073	25.088	17.162	0.453	1.00	27.54	8
ATOM	1904	N	CYS	1074	23.816	18.070	2.072	1.00	36.16	7
ATOM	1905	CA	CYS	1074	23.858	19.423	1.497	1.00	36.16	6
ATOM	1906	CB	CYS	1074	22.925	20.393	2.243	1.00	40.38	6
ATOM	1907	SG	CYS	1074	21.201	20.463	1.797	1.00	40.38	16
ATOM	1908	C	CYS	1074	25.282	19.995	1.627	1.00	36.16	6
ATOM	1909	O	CYS	1074	25.746	20.748	0.767	1.00	36.16	8
ATOM	1910	N	TRP	1075	25.958	19.619	2.716	1.00	26.48	7
ATOM	1911	CA	TRP	1075	27.302	20.120	3.049	1.00	26.48	6
ATOM	1912	CB	TRP	1075	27.413	20.389	4.570	1.00	32.15	6
ATOM	1913	CG	TRP	1075	26.260	21.224	5.181	1.00	32.15	6
ATOM	1914	CD2	TRP	1075	25.679	21.080	6.485	1.00	32.15	6
ATOM	1915	CE2	TRP	1075	24.682	22.075	6.613	1.00	32.15	6
ATOM	1916	CE3	TRP	1075	25.901	20.211	7.553	1.00	32.15	6
ATOM	1917	CD1	TRP	1075	25.607	22.272	4.597	1.00	32.15	6
ATOM	1918	NE1	TRP	1075	24.662	22.783	5.449	1.00	32.15	7
ATOM	1919	CZ2	TRP	1075	23.909	22.222	7.774	1.00	32.15	6
ATOM	1920	CZ3	TRP	1075	25.133	20.361	8.703	1.00	32.15	6
ATOM	1921	CH2	TRP	1075	24.148	21.357	8.807	1.00	32.15	6
ATOM	1922	C	TRP	1075	28.471	19.236	2.622	1.00	26.48	6
ATOM	1923	O	TRP	1075	29.599	19.447	3.071	1.00	26.48	8
ATOM	1924	N	ARG	1076	28.209	18.265	1.751	1.00	51.58	7
ATOM	1925	CA	ARG	1076	29.258	17.367	1.279	1.00	51.58	6
ATOM	1926	CB	ARG	1076	28.683	16.391	0.249	1.00	67.56	6

FIG. 3HH

ATOM	1927	CG	ARG	1076	27.618	15.509	0.847	1.00	67.56	6
ATOM	1928	CD	ARG	1076	27.279	14.291	0.009	1.00	67.56	6
ATOM	1929	NE	ARG	1076	26.267	13.485	0.690	1.00	67.56	7
ATOM	1930	CZ	ARG	1076	25.731	12.365	0.215	1.00	67.56	6
ATOM	1931	NH1	ARG	1076	26.104	11.891	-0.966	1.00	67.56	7
ATOM	1932	NH2	ARG	1076	24.819	11.714	0.929	1.00	67.56	7
ATOM	1933	C	ARG	1076	30.431	18.157	0.710	1.00	51.58	6
ATOM	1934	O	ARG	1076	30.238	19.206	0.103	1.00	51.58	8
ATOM	1935	N	GLU	1077	31.642	17.651	0.941	1.00	50.74	7
ATOM	1936	CA	GLU	1077	32.885	18.281	0.488	1.00	50.74	6
ATOM	1937	CB	GLU	1077	34.059	17.419	0.893	1.00	91.21	6
ATOM	1938	C	GLU	1077	32.927	18.540	-1.013	1.00	50.74	6
ATOM	1939	O	GLU	1077	33.213	19.657	-1.450	1.00	50.74	8
ATOM	1940	N	LYS	1078	32.656	17.494	-1.790	1.00	49.20	7
ATOM	1941	CA	LYS	1078	32.657	17.579	-3.240	1.00	49.20	6
ATOM	1942	CB	LYS	1078	32.895	16.197	-3.847	1.00	93.58	6
ATOM	1943	CG	LYS	1078	34.289	15.666	-3.640	1.00	93.51	6
ATOM	1944	CD	LYS	1078	34.458	14.341	-4.346	1.00	93.51	6
ATOM	1945	CE	LYS	1078	35.872	13.806	-4.191	1.00	93.51	6
ATOM	1946	NZ	LYS	1078	36.025	12.476	-4.860	1.00	93.51	7
ATOM	1947	C	LYS	1078	31.345	18.145	-3.760	1.00	49.20	6
ATOM	1948	O	LYS	1078	30.290	17.528	-3.617	1.00	49.20	8
ATOM	1949	N	PRO	1079	31.390	19.341	-4.366	1.00	30.47	7
ATOM	1950	CD	PRO	1079	32.592	20.190	-4.459	1.00	29.67	6
ATOM	1951	CA	PRO	1079	30.236	20.040	-4.931	1.00	30.47	6
ATOM	1952	CB	PRO	1079	30.887	21.098	-5.791	1.00	29.67	6
ATOM	1953	CG	PRO	1079	32.024	21.511	-4.914	1.00	29.67	6
ATOM	1954	C	PRO	1079	29.235	19.190	-5.711	1.00	30.47	6
ATOM	1955	O	PRO	1079	28.040	19.221	-5.420	1.00	30.47	8
ATOM	1956	N	TYR	1080	29.708	18.462	-6.718	1.00	44.53	7
ATOM	1957	CA	TYR	1080	28.821	17.616	-7.520	1.00	44.53	6
ATOM	1958	CB	TYR	1080	29.576	17.054	-8.730	1.00	62.16	6
ATOM	1959	CG	TYR	1080	30.938	16.479	-8.412	1.00	62.16	6
ATOM	1960	CD1	TYR	1080	31.072	15.207	-7.859	1.00	62.16	6
ATOM	1961	CE1	TYR	1080	32.329	14.691	-7.531	1.00	62.16	6
ATOM	1962	CD2	TYR	1080	32.095	17.223	-8.636	1.00	62.16	6
ATOM	1963	CE2	TYR	1080	33.351	16.722	-8.312	1.00	62.16	6
ATOM	1964	CZ	TYR	1080	33.462	15.458	-7.757	1.00	62.16	6
ATOM	1965	OH	TYR	1080	34.701	14.970	-7.409	1.00	62.16	8
ATOM	1966	C	TYR	1080	28.232	16.490	-6.672	1.00	44.53	6
ATOM	1967	O	TYR	1080	27.282	15.833	-7.087	1.00	44.53	8
ATOM	1968	N	GLU	1081	28.792	16.285	-5.484	1.00	41.53	7
ATOM	1969	CA	GLU	1081	28.285	15.257	-4.588	1.00	41.53	6
ATOM	1970	CB	GLU	1081	29.373	14.767	-3.638	1.00	60.45	6
ATOM	1971	CG	GLU	1081	30.292	13.713	-4.220	1.00	60.45	6
ATOM	1972	CD	GLU	1081	31.240	13.143	-3.182	1.00	60.45	6
ATOM	1973	OE1	GLU	1081	31.903	12.119	-3.470	1.00	60.45	8
ATOM	1974	OE2	GLU	1081	31.323	13.726	-2.079	1.00	60.45	8
ATOM	1975	C	GLU	1081	27.114	15.809	-3.778	1.00	41.53	6
ATOM	1976	O	GLU	1081	26.512	15.099	-2.972	1.00	41.53	8
ATOM	1977	N	ARG	1082	26.812	17.087	-3.975	1.00	50.75	7
ATOM	1978	CA	ARG	1082	25.702	17.706	-3.280	1.00	50.75	6
ATOM	1979	CB	ARG	1082	25.979	19.207	-3.053	1.00	30.76	6
ATOM	1980	CG	ARG	1082	26.429	19.535	-1.624	1.00	30.76	6
ATOM	1981	CD	ARG	1082	27.857	20.100	-1.505	1.00	30.76	6
ATOM	1982	NE	ARG	1082	27.939	21.540	-1.743	1.00	30.76	7
ATOM	1983	CZ	ARG	1082	29.060	22.258	-1.663	1.00	30.76	6

FIG. 3II

ATOM	1984	NH1	ARG	1082	30.225	21.698	-1.358	1.00	30.76	7
ATOM	1985	NH2	ARG	1082	29.007	23.567	-1.865	1.00	30.76	7
ATOM	1986	C	ARG	1082	24.446	17.479	-4.124	1.00	50.75	6
ATOM	1987	O	ARG	1082	24.501	17.497	-5.355	1.00	50.75	8
ATOM	1988	N	PRO	1083	23.303	17.225	-3.464	1.00	42.97	7
ATOM	1989	CD	PRO	1083	23.155	17.153	-1.995	1.00	16.51	6
ATOM	1990	CA	PRO	1083	22.022	16.983	-4.127	1.00	42.97	6
ATOM	1991	CB	PRO	1083	21.171	16.382	-3.015	1.00	16.51	6
ATOM	1992	CG	PRO	1083	21.665	17.079	-1.805	1.00	16.51	6
ATOM	1993	C	PRO	1083	21.450	18.268	-4.715	1.00	42.97	6
ATOM	1994	O	PRO	1083	21.914	19.353	-4.402	1.00	42.97	8
ATOM	1995	N	SER	1084	20.448	18.132	-5.564	1.00	43.29	7
ATOM	1996	CA	SER	1084	19.842	19.275	-6.217	1.00	43.29	6
ATOM	1997	CB	SER	1084	19.553	18.890	-7.643	1.00	28.32	6
ATOM	1998	OG	SER	1084	18.965	17.607	-7.610	1.00	28.32	8
ATOM	1999	C	SER	1084	18.543	19.679	-5.538	1.00	43.29	6
ATOM	2000	O	SER	1084	17.901	18.858	-4.878	1.00	43.29	8
ATOM	2001	N	PHE	1085	18.148	20.934	-5.723	1.00	22.83	7
ATOM	2002	CA	PHE	1085	16.913	21.427	-5.128	1.00	22.83	6
ATOM	2003	CB	PHE	1085	16.688	22.881	-5.538	1.00	7.27	6
ATOM	2004	CG	PHE	1085	17.599	23.814	-4.858	1.00	7.27	6
ATOM	2005	CD1	PHE	1085	18.487	24.598	-5.588	1.00	7.27	6
ATOM	2006	CD2	PHE	1085	17.592	23.899	-3.476	1.00	7.27	6
ATOM	2007	CE1	PHE	1085	19.356	25.462	-4.949	1.00	7.27	6
ATOM	2008	CE2	PHE	1085	18.454	24.756	-2.819	1.00	7.27	6
ATOM	2009	CZ	PHE	1085	19.341	25.545	-3.560	1.00	7.27	6
ATOM	2010	C	PHE	1085	15.710	20.587	-5.510	1.00	22.83	6
ATOM	2011	O	PHE	1085	14.660	20.668	-4.882	1.00	22.83	8
ATOM	2012	N	ALA	1086	15.878	19.789	-6.553	1.00	45.86	7
ATOM	2013	CA	ALA	1086	14.813	18.919	-7.016	1.00	45.86	6
ATOM	2014	CB	ALA	1086	15.037	18.540	-8.430	1.00	15.16	6
ATOM	2015	C	ALA	1086	14.783	17.674	-6.161	1.00	45.86	6
ATOM	2016	O	ALA	1086	13.720	17.175	-5.815	1.00	45.86	8
ATOM	2017	N	GLN	1087	15.959	17.180	-5.810	1.00	32.39	7
ATOM	2018	CA	GLN	1087	16.020	15.990	-5.000	1.00	32.39	6
ATOM	2019	CB	GLN	1087	17.433	15.386	-5.038	1.00	50.88	6
ATOM	2020	CG	GLN	1087	17.971	15.230	-6.466	1.00	50.88	6
ATOM	2021	CD	GLN	1087	19.290	14.488	-6.552	1.00	50.88	6
ATOM	2022	OE1	GLN	1087	20.221	14.752	-5.790	1.00	50.88	8
ATOM	2023	NE2	GLN	1087	19.389	13.577	-7.510	1.00	50.88	7
ATOM	2024	C	GLN	1087	15.617	16.398	-3.592	1.00	32.39	6
ATOM	2025	O	GLN	1087	14.792	15.737	-2.956	1.00	32.39	8
ATOM	2026	N	ILE	1088	16.177	17.507	-3.116	1.00	19.40	7
ATOM	2027	CA	ILE	1088	15.875	17.997	-1.761	1.00	19.40	6
ATOM	2028	CB	ILE	1088	16.519	19.358	-1.532	1.00	20.50	6
ATOM	2029	CG2	ILE	1088	16.172	19.905	-0.185	1.00	20.50	6
ATOM	2030	CG1	ILE	1088	18.017	19.199	-1.630	1.00	20.50	6
ATOM	2031	CD1	ILE	1088	18.747	20.459	-1.361	1.00	20.50	6
ATOM	2032	C	ILE	1088	14.375	18.102	-1.531	1.00	19.40	6
ATOM	2033	O	ILE	1088	13.852	17.646	-0.514	1.00	19.40	8
ATOM	2034	N	LEU	1089	13.697	18.700	-2.500	1.00	31.43	7
ATOM	2035	CA	LEU	1089	12.262	18.860	-2.452	1.00	31.43	6
ATOM	2036	CB	LEU	1089	11.783	19.531	-3.714	1.00	14.58	6
ATOM	2037	CG	LEU	1089	10.376	20.070	-3.576	1.00	14.58	6
ATOM	2038	CD1	LEU	1089	10.208	20.858	-2.288	1.00	14.58	6
ATOM	2039	CD2	LEU	1089	10.136	20.941	-4.788	1.00	14.58	6
ATOM	2040	C	LEU	1089	11.595	17.509	-2.335	1.00	31.43	6

FIG. 3JJ

ATOM	2041	O	LEU	1089	10.804	17.270	-1.423	1.00	31.43	8
ATOM	2042	N	VAL	1090	11.920	16.619	-3.265	1.00	26.46	7
ATOM	2043	CA	VAL	1090	11.346	15.288	-3.242	1.00	26.46	6
ATOM	2044	CB	VAL	1090	12.042	14.338	-4.171	1.00	24.17	6
ATOM	2045	CG1	VAL	1090	11.419	12.957	-4.012	1.00	24.17	6
ATOM	2046	CG2	VAL	1090	11.913	14.819	-5.581	1.00	24.17	6
ATOM	2047	C	VAL	1090	11.441	14.697	-1.861	1.00	26.46	6
ATOM	2048	O	VAL	1090	10.476	14.126	-1.362	1.00	26.46	8
ATOM	2049	N	SER	1091	12.600	14.819	-1.235	1.00	24.68	7
ATOM	2050	CA	SER	1091	12.726	14.276	0.094	1.00	24.68	6
ATOM	2051	CB	SER	1091	14.156	14.407	0.599	1.00	45.28	6
ATOM	2052	OG	SER	1091	15.039	13.699	-0.249	1.00	45.28	8
ATOM	2053	C	SER	1091	11.742	14.999	1.006	1.00	24.68	6
ATOM	2054	O	SER	1091	10.796	14.379	1.471	1.00	24.68	8
ATOM	2055	N	LEU	1092	11.919	16.302	1.231	1.00	45.44	7
ATOM	2056	CA	LEU	1092	11.001	17.031	2.112	1.00	45.44	6
ATOM	2057	CB	LEU	1092	11.127	18.557	1.905	1.00	19.86	6
ATOM	2058	CG	LEU	1092	12.518	19.144	2.242	1.00	19.86	6
ATOM	2059	CD1	LEU	1092	12.611	20.594	1.810	1.00	19.86	6
ATOM	2060	CD2	LEU	1092	12.793	19.007	3.728	1.00	19.86	6
ATOM	2061	C	LEU	1092	9.554	16.568	1.918	1.00	45.44	6
ATOM	2062	O	LEU	1092	8.821	16.438	2.891	1.00	45.44	8
ATOM	2063	N	ASN	1093	9.162	16.275	0.678	1.00	44.52	7
ATOM	2064	CA	ASN	1093	7.797	15.820	0.360	1.00	44.52	6
ATOM	2065	CB	ASN	1093	7.578	15.906	-1.147	1.00	34.39	6
ATOM	2066	CG	ASN	1093	7.266	17.302	-1.586	1.00	34.39	6
ATOM	2067	OD1	ASN	1093	7.572	17.705	-2.703	1.00	34.39	8
ATOM	2068	ND2	ASN	1093	6.639	18.061	-0.698	1.00	34.39	7
ATOM	2069	C	ASN	1093	7.501	14.414	0.849	1.00	44.52	6
ATOM	2070	O	ASN	1093	6.437	14.137	1.401	1.00	44.52	8
ATOM	2071	N	ARG	1094	8.458	13.529	0.631	1.00	42.85	7
ATOM	2072	CA	ARG	1094	8.329	12.168	1.074	1.00	42.85	6
ATOM	2073	CB	ARG	1094	9.491	11.353	0.472	1.00	83.86	6
ATOM	2074	CG	ARG	1094	10.129	10.325	1.373	1.00	83.62	6
ATOM	2075	CD	ARG	1094	11.099	10.992	2.328	1.00	83.62	6
ATOM	2076	NE	ARG	1094	11.576	10.076	3.359	1.00	83.62	7
ATOM	2077	CZ	ARG	1094	10.787	9.365	4.163	1.00	83.62	6
ATOM	2078	NH1	ARG	1094	9.466	9.461	4.070	1.00	83.62	7
ATOM	2079	NH2	ARG	1094	11.323	8.549	5.061	1.00	83.62	7
ATOM	2080	C	ARG	1094	8.293	12.166	2.628	1.00	42.85	6
ATOM	2081	O	ARG	1094	7.667	11.308	3.239	1.00	42.85	8
ATOM	2082	N	MET	1095	8.934	13.151	3.253	1.00	51.73	7
ATOM	2083	CA	MET	1095	8.991	13.279	4.712	1.00	51.73	6
ATOM	2084	CB	MET	1095	10.206	14.135	5.109	1.00	28.03	6
ATOM	2085	CG	MET	1095	11.242	13.507	5.999	1.00	28.03	6
ATOM	2086	SD	MET	1095	12.707	14.551	6.044	1.00	28.03	16
ATOM	2087	CE	MET	1095	13.094	14.706	4.302	1.00	28.03	6
ATOM	2088	C	MET	1095	7.757	13.989	5.274	1.00	51.73	6
ATOM	2089	O	MET	1095	7.425	13.870	6.450	1.00	51.73	8
ATOM	2090	N	LEU	1096	7.123	14.763	4.413	1.00	48.50	7
ATOM	2091	CA	LEU	1096	5.981	15.557	4.825	1.00	48.50	6
ATOM	2092	CB	LEU	1096	5.889	16.790	3.951	1.00	41.93	6
ATOM	2093	CG	LEU	1096	6.365	18.048	4.638	1.00	41.93	6
ATOM	2094	CD1	LEU	1096	6.177	19.139	3.616	1.00	41.93	6
ATOM	2095	CD2	LEU	1096	5.593	18.342	5.911	1.00	41.93	6
ATOM	2096	C	LEU	1096	4.663	14.859	4.783	1.00	48.50	6
ATOM	2097	O	LEU	1096	3.747	15.199	5.536	1.00	48.50	8

FIG. 3KK

ATOM	2098	N	GLU	1097	4.537	13.900	3.890	1.00	62.96	7
ATOM	2099	CA	GLU	1097	3.261	13.252	3.809	1.00	63.28	6
ATOM	2100	CB	GLU	1097	3.046	12.672	2.424	1.00	90.58	6
ATOM	2101	CG	GLU	1097	2.625	13.708	1.449	1.00	90.58	6
ATOM	2102	CD	GLU	1097	2.523	13.139	0.080	1.00	90.58	6
ATOM	2103	OE1	GLU	1097	3.480	12.481	-0.333	1.00	90.58	8
ATOM	2104	OE2	GLU	1097	1.492	13.317	-0.587	1.00	90.58	8
ATOM	2105	C	GLU	1097	3.099	12.216	4.892	1.00	64.94	6
ATOM	2106	O	GLU	1097	2.839	11.051	4.616	1.00	67.39	8
ATOM	2107	N	GLU	1098	3.279	12.659	6.137	1.00	99.89	7
ATOM	2108	CA	GLU	1098	3.132	11.782	7.288	1.00	99.89	6
ATOM	2109	CB	GLU	1098	4.342	10.880	7.434	1.00	62.46	6
ATOM	2110	CG	GLU	1098	4.908	10.367	6.157	1.00	62.46	6
ATOM	2111	CD	GLU	1098	6.147	9.556	6.415	1.00	62.46	6
ATOM	2112	OE1	GLU	1098	6.614	9.586	7.576	1.00	62.46	8
ATOM	2113	OE2	GLU	1098	6.653	8.914	5.474	1.00	62.46	8
ATOM	2114	C	GLU	1098	2.928	12.540	8.608	1.00	99.89	6
ATOM	2115	O	GLU	1098	1.962	12.277	9.312	1.00	99.89	8
ATOM	2116	N	ARG	1099	3.815	13.483	8.937	1.00	100.00	7
ATOM	2117	CA	ARG	1099	3.735	14.251	10.201	1.00	100.00	6
ATOM	2118	CB	ARG	1099	2.339	14.863	10.443	1.00	95.05	6
ATOM	2119	CG	ARG	1099	2.140	15.416	11.871	1.00	83.68	6
ATOM	2120	CD	ARG	1099	3.239	16.413	12.239	1.00	83.68	6
ATOM	2121	NE	ARG	1099	3.123	16.915	13.609	1.00	83.68	7
ATOM	2122	CZ	ARG	1099	3.314	18.185	13.955	1.00	83.68	6
ATOM	2123	NH1	ARG	1099	3.636	19.072	13.024	1.00	83.68	7
ATOM	2124	NH2	ARG	1099	3.179	18.572	15.222	1.00	83.68	7
ATOM	2125	C	ARG	1099	4.083	13.322	11.354	1.00	100.00	6
ATOM	2126	O	ARG	1099	3.393	13.259	12.370	1.00	100.00	8
ATOM	2127	N	LYS	1100	5.153	12.570	11.174	1.00	88.41	7
ATOM	2128	CA	LYS	1100	5.572	11.681	12.224	1.00	88.41	6
ATOM	2129	CB	LYS	1100	6.250	10.454	11.641	1.00	87.41	6
ATOM	2130	CG	LYS	1100	5.322	9.628	10.762	1.00	87.41	6
ATOM	2131	CD	LYS	1100	3.984	9.336	11.456	1.00	87.41	6
ATOM	2132	CE	LYS	1100	4.165	8.742	12.861	1.00	59.92	6
ATOM	2133	NZ	LYS	1100	4.852	7.411	12.877	1.00	59.92	7
ATOM	2134	C	LYS	1100	6.519	12.453	13.123	1.00	88.41	6
ATOM	2135	O	LYS	1100	7.597	11.969	13.470	1.00	88.41	8
ATOM	2136	N	THR	1101	6.112	13.672	13.472	1.00	100.00	7
ATOM	2137	CA	THR	1101	6.892	14.519	14.356	1.00	100.00	6
ATOM	2138	CB	THR	1101	6.795	13.998	15.811	1.00	100.00	6
ATOM	2139	OG1	THR	1101	5.426	14.034	16.239	1.00	90.24	8
ATOM	2140	CG2	THR	1101	7.652	14.836	16.750	1.00	90.24	6
ATOM	2141	C	THR	1101	8.362	14.565	13.927	1.00	100.00	6
ATOM	2142	O	THR	1101	9.219	13.923	14.541	1.00	100.00	8
ATOM	2143	N	TYR	1102	8.655	15.300	12.862	1.00	39.18	7
ATOM	2144	CA	TYR	1102	10.042	15.411	12.416	1.00	39.18	6
ATOM	2145	CB	TYR	1102	10.106	15.624	10.912	1.00	91.13	6
ATOM	2146	CG	TYR	1102	9.798	14.391	10.132	1.00	60.67	6
ATOM	2147	CD1	TYR	1102	8.500	14.112	9.717	1.00	60.67	6
ATOM	2148	CE1	TYR	1102	8.222	12.956	9.006	1.00	60.67	6
ATOM	2149	CD2	TYR	1102	10.809	13.487	9.821	1.00	60.67	6
ATOM	2150	CE2	TYR	1102	10.544	12.338	9.120	1.00	60.67	6
ATOM	2151	CZ	TYR	1102	9.256	12.078	8.711	1.00	60.67	6
ATOM	2152	OH	TYR	1102	9.019	10.950	7.978	1.00	60.67	8
ATOM	2153	C	TYR	1102	10.781	16.549	13.102	1.00	39.18	6
ATOM	2154	O	TYR	1102	12.003	16.594	13.090	1.00	39.18	8

FIG. 3LL

ATOM	2155	N	VAL	1103	10.028	17.469	13.690	1.00	80.69	7
ATOM	2156	CA	VAL	1103	10.614	18.614	14.370	1.00	80.69	6
ATOM	2157	CB	VAL	1103	10.585	19.857	13.466	1.00	82.85	6
ATOM	2158	CG1	VAL	1103	11.221	21.042	14.165	1.00	25.69	6
ATOM	2159	CG2	VAL	1103	11.310	19.563	12.172	1.00	25.69	6
ATOM	2160	C	VAL	1103	9.791	18.892	15.611	1.00	80.69	6
ATOM	2161	O	VAL	1103	8.677	19.395	15.529	1.00	80.69	8
ATOM	2162	N	ASN	1104	10.345	18.570	16.767	1.00	61.67	7
ATOM	2163	CA	ASN	1104	9.624	18.773	18.003	1.00	61.67	6
ATOM	2164	CB	ASN	1104	10.315	18.015	19.112	1.00	93.99	6
ATOM	2165	CG	ASN	1104	9.344	17.404	20.054	1.00	53.82	6
ATOM	2166	OD1	ASN	1104	8.643	18.111	20.791	1.00	53.82	8
ATOM	2167	ND2	ASN	1104	9.261	16.076	20.028	1.00	53.82	7
ATOM	2168	C	ASN	1104	9.470	20.240	18.395	1.00	61.67	6
ATOM	2169	O	ASN	1104	10.453	20.966	18.484	1.00	61.67	8
ATOM	2170	N	THR	1105	8.233	20.675	18.625	1.00	43.79	7
ATOM	2171	CA	THR	1105	7.960	22.059	19.024	1.00	43.79	6
ATOM	2172	CB	THR	1105	7.081	22.763	18.002	1.00	95.52	6
ATOM	2173	OG1	THR	1105	5.888	22.001	17.786	1.00	51.15	8
ATOM	2174	CG2	THR	1105	7.835	22.923	16.700	1.00	51.15	6
ATOM	2175	C	THR	1105	7.231	22.045	20.350	1.00	43.79	6
ATOM	2176	O	THR	1105	6.598	23.024	20.754	1.00	43.79	8
ATOM	2177	N	THR	1106	7.338	20.905	21.016	1.00	47.73	7
ATOM	2178	CA	THR	1106	6.683	20.671	22.281	1.00	47.73	6
ATOM	2179	CB	THR	1106	5.850	19.415	22.236	1.00	24.03	6
ATOM	2180	OG1	THR	1106	4.835	19.542	21.237	1.00	24.03	8
ATOM	2181	CG2	THR	1106	5.222	19.167	23.580	1.00	24.03	6
ATOM	2182	C	THR	1106	7.676	20.434	23.372	1.00	47.73	6
ATOM	2183	O	THR	1106	8.742	19.880	23.129	1.00	47.73	8
ATOM	2184	N	LEU	1107	7.311	20.833	24.583	1.00	64.31	7
ATOM	2185	CA	LEU	1107	8.174	20.612	25.723	1.00	64.31	6
ATOM	2186	CB	LEU	1107	8.207	21.803	26.637	1.00	96.32	6
ATOM	2187	CG	LEU	1107	8.957	22.900	25.957	1.00	40.62	6
ATOM	2188	CD1	LEU	1107	7.919	23.838	25.432	1.00	40.62	6
ATOM	2189	CD2	LEU	1107	9.864	23.587	26.914	1.00	40.62	6
ATOM	2190	C	LEU	1107	7.795	19.433	26.564	1.00	64.31	6
ATOM	2191	O	LEU	1107	6.801	19.458	27.281	1.00	64.31	8
ATOM	2192	N	TYR	1108	8.708	18.463	26.384	1.00	94.02	7
ATOM	2193	CA	TYR	1108	8.405	17.305	27.238	1.00	94.02	6
ATOM	2194	CB	TYR	1108	8.596	16.009	26.448	1.00	99.65	6
ATOM	2195	CG	TYR	1108	7.705	15.929	25.207	1.00	78.77	6
ATOM	2196	CD1	TYR	1108	7.913	14.643	24.404	1.00	78.77	6
ATOM	2197	CD2	TYR	1108	6.212	15.974	25.538	1.00	78.77	6
ATOM	2198	C	TYR	1108	9.340	17.291	28.449	1.00	94.02	6
ATOM	2199	O	TYR	1108	8.922	16.976	29.574	1.00	94.02	8
ATOM	2200	N	GLU	1109	10.796	17.582	27.521	1.00	92.55	7
ATOM	2201	CA	GLU	1109	11.496	17.815	28.793	1.00	92.55	6
ATOM	2202	CB	GLU	1109	11.234	16.655	29.755	1.00	95.82	6
ATOM	2203	C	GLU	1109	13.002	17.927	28.549	1.00	92.55	6
ATOM	2204	O	GLU	1109	13.672	16.935	28.226	1.00	92.55	8
ATOM	2205	N	LYS	1110	13.581	19.231	28.669	1.00	54.62	7
ATOM	2206	CA	LYS	1110	14.995	19.556	28.430	1.00	54.62	6
ATOM	2207	CB	LYS	1110	15.850	18.294	28.564	1.00	100.00	6
ATOM	2208	CG	LYS	1110	16.129	17.914	30.020	1.00	99.80	6
ATOM	2209	CD	LYS	1110	17.313	16.956	30.171	1.00	99.80	6
ATOM	2210	CE	LYS	1110	17.333	16.240	31.523	1.00	99.80	6
ATOM	2211	NZ	LYS	1110	18.525	15.400	31.710	1.00	99.80	7

FIG. 3MM

```
ATOM   2212  C   LYS  1110      15.168  20.134  27.023  1.00 54.62   6
ATOM   2213  O   LYS  1110      15.875  19.561  26.181  1.00 54.62   8
ATOM   2214  N   PHE  1111      14.506  21.258  26.825  1.00 53.78   7
ATOM   2215  CA  PHE  1111      14.527  21.994  25.551  1.00 53.78   6
ATOM   2216  CB  PHE  1111      13.134  22.558  25.259  1.00 97.53   6
ATOM   2217  CG  PHE  1111      12.847  22.718  23.764  1.00 42.19   6
ATOM   2218  CD1 PHE  1111      12.368  21.631  23.023  1.00 42.19   6
ATOM   2219  CD2 PHE  1111      13.062  23.951  23.140  1.00 42.19   6
ATOM   2220  CE1 PHE  1111      12.104  21.779  21.655  1.00 42.19   6
ATOM   2221  CE2 PHE  1111      12.798  24.100  21.773  1.00 42.19   6
ATOM   2222  CZ  PHE  1111      12.318  23.013  21.031  1.00 42.19   6
ATOM   2223  C   PHE  1111      15.528  23.149  25.640  1.00 53.78   6
ATOM   2224  O   PHE  1111      15.647  23.812  26.681  1.00 53.78   8
ATOM   2225  N   THR  1112      16.171  23.593  24.331  1.00 41.67   7
ATOM   2226  CA  THR  1112      17.246  24.596  24.296  1.00 41.67   6
ATOM   2227  CB  THR  1112      18.609  23.900  24.280  1.00 81.18   6
ATOM   2228  OG1 THR  1112      18.657  22.952  23.224  1.00 45.38   8
ATOM   2229  CG2 THR  1112      18.915  23.153  25.579  1.00 45.38   6
ATOM   2230  C   THR  1112      17.113  25.461  23.041  1.00 41.67   6
ATOM   2231  O   THR  1112      16.476  25.063  22.055  1.00 41.67   8
ATOM   2232  N   TYR  1113      17.727  26.628  23.125  1.00 88.60   7
ATOM   2233  CA  TYR  1113      17.729  27.614  22.034  1.00 88.60   6
ATOM   2234  CB  TYR  1113      16.857  28.816  22.408  1.00 72.51   6
ATOM   2235  CG  TYR  1113      15.375  28.464  22.561  1.00 11.65   6
ATOM   2236  CD1 TYR  1113      14.778  28.484  23.827  1.00 11.65   6
ATOM   2237  CE1 TYR  1113      13.422  28.166  23.967  1.00 11.65   6
ATOM   2238  CD2 TYR  1113      14.614  28.124  21.435  1.00 11.65   6
ATOM   2239  CE2 TYR  1113      13.258  27.806  21.575  1.00 11.65   6
ATOM   2240  CZ  TYR  1113      12.662  27.827  22.842  1.00 11.65   6
ATOM   2241  OH  TYR  1113      11.344  27.518  22.978  1.00 11.65   8
ATOM   2242  C   TYR  1113      19.155  28.108  21.772  1.00 88.60   6
ATOM   2243  O   TYR  1113      20.133  27.378  21.991  1.00 88.60   8
ATOM   2244  N   ALA  1114      19.217  29.344  21.309  1.00 62.73   7
ATOM   2245  CA  ALA  1114      20.484  30.020  20.989  1.00 62.73   6
ATOM   2246  CB  ALA  1114      21.530  28.992  20.552  1.00  7.22   6
ATOM   2247  C   ALA  1114      20.268  31.024  19.854  1.00 62.73   6
ATOM   2248  O   ALA  1114      20.108  30.642  18.685  1.00 62.73   8
ATOM   2249  N   GLY  1115      20.271  32.287  20.241  1.00 60.96   7
ATOM   2250  CA  GLY  1115      20.078  33.409  19.310  1.00 60.96   6
ATOM   2251  C   GLY  1115      21.034  34.552  19.657  1.00 60.96   6
ATOM   2252  O   GLY  1115      20.817  35.296  20.625  1.00 60.96   8
ATOM   2253  N   ILE  1116      22.069  34.651  18.843  1.00 82.32   7
ATOM   2254  CA  ILE  1116      23.110  35.679  18.992  1.00 82.32   6
ATOM   2255  CB  ILE  1116      22.488  37.073  18.892  1.00 68.50   6
ATOM   2256  C   ILE  1116      23.796  35.537  20.352  1.00 82.32   6
ATOM   2257  O   ILE  1116      24.984  35.192  20.436  1.00 82.32   8
ATOM   2258  OXT ILE  1116      23.443  36.522  21.208  1.00 64.86   8
TER
HETATM 2259  C29 TEM     1      14.137  43.777  -1.896  1.00 87.75   6
HETATM 2260  C30 TEM     1      15.517  44.384  -2.200  1.00 92.68   9
HETATM 2261  C31 TEM     1      13.532  43.986  -0.603  1.00 84.61   6
HETATM 2262  C32 TEM     1      10.062  43.539   1.417  1.00 72.29   6
HETATM 2263  C28 TEM     1      13.152  42.505  -7.029  1.00 92.68   6
HETATM 2264  C8  TEM     1      11.669  44.356   4.626  1.00 64.60   6
HETATM 2265  C9  TEM     1      12.234  43.146   5.418  1.00 62.65   6
HETATM 2266  C10 TEM     1      12.979  43.794   6.609  1.00 61.60   6
HETATM 2267  C11 TEM     1      13.328  45.233   6.175  1.00 61.11   6
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FIG. 3NN

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HETATM 2268  C12 TEM     1      12.788  45.420   4.740  1.00 62.68   6
HETATM 2269  C13 TEM     1      12.175  43.912   2.185  1.00 71.00   6
HETATM 2270  N7  TEM     1      11.303  44.043   3.228  1.00 67.78   7
HETATM 2271  N1  TEM     1       8.672  43.004  -0.559  1.00 73.02   7
HETATM 2272  C2  TEM     1       8.784  43.270   0.784  1.00 71.64   6
HETATM 2273  N3  TEM     1       7.669  43.306   1.546  1.00 71.42   7
HETATM 2274  C4  TEM     1       7.718  43.568   2.851  1.00 69.68   6
HETATM 2275  N5  TEM     1       8.853  43.811   3.473  1.00 68.84   7
HETATM 2276  C6  TEM     1      10.030  43.817   2.820  1.00 69.92   6
HETATM 2277  C14 TEM     1      11.530  43.630   1.036  1.00 75.68   6
HETATM 2278  O22 TEM     1      13.956  40.236  -4.115  1.00 92.68   8
HETATM 2279  C23 TEM     1      13.420  41.285  -6.355  1.00 92.68   6
HETATM 2280  C24 TEM     1      12.844  40.071  -6.856  1.00 92.68   6
HETATM 2281  C25 TEM     1      12.014  40.102  -8.027  1.00 92.68   6
HETATM 2282  C26 TEM     1      11.757  41.334  -8.689  1.00 92.68   6
HETATM 2283  C27 TEM     1      12.330  42.534  -8.187  1.00 92.68   6
HETATM 2284  O21 TEM     1      15.786  41.592  -5.276  1.00 92.68   8
HETATM 2285  C15 TEM     1      12.216  43.429  -0.313  1.00 80.63   6
HETATM 2286  C16 TEM     1      11.576  42.675  -1.308  1.00 83.45   6
HETATM 2287  C17 TEM     1      12.141  42.492  -2.551  1.00 87.27   6
HETATM 2288  C18 TEM     1      13.399  43.018  -2.887  1.00 88.78   6
HETATM 2289  N19 TEM     1      13.818  42.732  -4.220  1.00 90.27   7
HETATM 2290  S20 TEM     1      14.444  41.335  -4.875  1.00 92.68  16
ATOM   2291  S   SO4     2      25.361  40.893  -8.736  1.00 15.55  16
ATOM   2292  O1  SO4     2      26.331  39.742  -8.499  1.00 20.26   8
ATOM   2293  O2  SO4     2      25.230  41.131 -10.222  1.00 12.30   8
ATOM   2294  O3  SO4     2      23.982  40.607  -8.171  1.00 16.39   8
ATOM   2295  O4  SO4     2      25.930  42.110  -8.051  1.00 17.72   8
END
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FIG. 300

ATOM	1	N	VAL	A	818	77.669	47.027	2.354	1.00 20.00
ATOM	2	CA	VAL	A	818	76.422	47.479	1.690	1.00 20.00
ATOM	3	C	VAL	A	818	75.257	46.471	1.737	1.00 20.00
ATOM	4	O	VAL	A	818	75.361	45.363	2.335	1.00 20.00
ATOM	5	CB	VAL	A	818	76.716	47.863	0.250	1.00 20.00
ATOM	9	N	LEU	A	819	74.145	46.870	1.095	1.00 20.00
ATOM	10	CA	LEU	A	819	72.922	46.055	1.058	1.00 20.00
ATOM	11	C	LEU	A	819	72.341	45.959	-0.347	1.00 20.00
ATOM	12	O	LEU	A	819	71.187	46.223	-0.571	1.00 20.00
ATOM	13	CB	LEU	A	819	71.897	46.637	2.052	1.00 20.00
ATOM	14	CG	LEU	A	819	70.399	46.340	1.987	1.00 20.00
ATOM	15	CD1	LEU	A	819	70.026	45.327	3.039	1.00 20.00
ATOM	16	CD2	LEU	A	819	69.612	47.643	2.186	1.00 20.00
ATOM	18	N	ASP	A	820	73.165	45.565	-1.294	1.00 20.00
ATOM	19	CA	ASP	A	820	72.758	45.427	-2.685	1.00 20.00
ATOM	20	C	ASP	A	820	71.419	45.961	-3.188	1.00 20.00
ATOM	21	O	ASP	A	820	70.510	45.182	-3.445	1.00 20.00
ATOM	22	CB	ASP	A	820	72.867	43.971	-3.103	1.00 20.00
ATOM	23	CG	ASP	A	820	72.637	43.799	-4.570	1.00 20.00
ATOM	24	OD1	ASP	A	820	72.617	42.622	-5.045	1.00 20.00
ATOM	25	OD2	ASP	A	820	72.468	44.861	-5.242	1.00 20.00
ATOM	27	N	TRP	A	821	71.336	47.280	-3.390	1.00 20.00
ATOM	28	CA	TRP	A	821	70.128	47.958	-3.916	1.00 20.00
ATOM	29	C	TRP	A	821	69.296	47.063	-4.814	1.00 20.00
ATOM	30	O	TRP	A	821	68.077	47.237	-4.938	1.00 20.00
ATOM	31	CB	TRP	A	821	70.479	49.190	-4.782	1.00 20.00
ATOM	32	CG	TRP	A	821	69.336	50.211	-4.771	1.00 20.00
ATOM	33	CD1	TRP	A	821	68.872	50.892	-3.675	1.00 20.00
ATOM	34	CD2	TRP	A	821	68.465	50.552	-5.841	1.00 20.00
ATOM	35	NE1	TRP	A	821	67.753	51.628	-4.001	1.00 20.00
ATOM	36	CE2	TRP	A	821	67.482	51.435	-5.325	1.00 20.00
ATOM	37	CE3	TRP	A	821	68.408	50.201	-7.177	1.00 20.00
ATOM	38	CZ2	TRP	A	821	66.462	51.963	-6.104	1.00 20.00
ATOM	39	CZ3	TRP	A	821	67.382	50.730	-7.962	1.00 20.00
ATOM	40	CH2	TRP	A	821	66.430	51.597	-7.420	1.00 20.00
ATOM	43	N	ASN	A	822	69.999	46.156	-5.498	1.00 20.00
ATOM	44	CA	ASN	A	822	69.370	45.213	-6.404	1.00 20.00
ATOM	45	C	ASN	A	822	67.947	44.823	-5.911	1.00 20.00
ATOM	46	O	ASN	A	822	67.000	44.734	-6.707	1.00 20.00
ATOM	47	CB	ASN	A	822	70.291	43.986	-6.531	1.00 20.00
ATOM	48	CG	ASN	A	822	69.610	42.766	-7.181	1.00 20.00
ATOM	49	OD1	ASN	A	822	69.287	42.766	-8.393	1.00 20.00
ATOM	50	ND2	ASN	A	822	69.406	41.706	-6.377	1.00 20.00
ATOM	54	N	ASP	A	823	67.778	44.632	-4.602	1.00 20.00
ATOM	55	CA	ASP	A	823	66.472	44.212	-4.129	1.00 20.00
ATOM	56	C	ASP	A	823	65.921	44.808	-2.847	1.00 20.00
ATOM	57	O	ASP	A	823	66.179	44.295	-1.758	1.00 20.00
ATOM	58	CB	ASP	A	823	66.454	42.681	-4.008	1.00 20.00
ATOM	60	N	ILE	A	824	65.166	45.894	-2.988	1.00 20.00
ATOM	61	CA	ILE	A	824	64.480	46.524	-1.859	1.00 20.00
ATOM	62	C	ILE	A	824	63.021	46.501	-2.412	1.00 20.00
ATOM	63	O	ILE	A	824	62.776	46.906	-3.570	1.00 20.00
ATOM	64	CB	ILE	A	824	64.955	48.019	-1.586	1.00 20.00
ATOM	65	CG1	ILE	A	824	65.666	48.576	-2.803	1.00 20.00
ATOM	66	CG2	ILE	A	824	65.845	48.113	-0.382	1.00 20.00
ATOM	67	CD1	ILE	A	824	67.135	48.549	-2.681	1.00 20.00

FIG. 4A

```
ATOM     69  N   LYS A 825      62.077  45.969  -1.626  1.00 20.00
ATOM     70  CA  LYS A 825      60.645  45.921  -2.029  1.00 20.00
ATOM     71  C   LYS A 825      59.922  47.060  -1.266  1.00 20.00
ATOM     72  O   LYS A 825      59.578  46.946  -0.097  1.00 20.00
ATOM     73  CB  LYS A 825      60.043  44.561  -1.696  1.00 20.00
ATOM     75  N   PHE A 826      59.696  48.147  -1.988  1.00 20.00
ATOM     76  CA  PHE A 826      59.153  49.401  -1.462  1.00 20.00
ATOM     77  C   PHE A 826      57.643  49.569  -1.593  1.00 20.00
ATOM     78  O   PHE A 826      57.160  50.073  -2.593  1.00 20.00
ATOM     79  CB  PHE A 826      59.882  50.481  -2.224  1.00 20.00
ATOM     80  CG  PHE A 826      60.298  50.013  -3.604  1.00 20.00
ATOM     81  CD1 PHE A 826      59.336  49.841  -4.613  1.00 20.00
ATOM     82  CD2 PHE A 826      61.611  49.711  -3.887  1.00 20.00
ATOM     83  CE1 PHE A 826      59.675  49.383  -5.876  1.00 20.00
ATOM     84  CE2 PHE A 826      61.960  49.249  -5.145  1.00 20.00
ATOM     85  CZ  PHE A 826      60.984  49.086  -6.144  1.00 20.00
ATOM     87  N   GLN A 827      56.919  49.173  -0.550  1.00 20.00
ATOM     88  CA  GLN A 827      55.459  49.206  -0.491  1.00 20.00
ATOM     89  C   GLN A 827      54.788  50.547  -0.268  1.00 20.00
ATOM     90  O   GLN A 827      54.134  51.071  -1.177  1.00 20.00
ATOM     91  CB  GLN A 827      54.978  48.268   0.591  1.00 20.00
ATOM     92  CG  GLN A 827      56.111  47.581   1.340  1.00 20.00
ATOM     93  CD  GLN A 827      56.511  46.315   0.637  1.00 20.00
ATOM     94  OE1 GLN A 827      56.636  45.253   1.256  1.00 20.00
ATOM     95  NE2 GLN A 827      56.688  46.410  -0.675  1.00 20.00
ATOM     99  N   ASP A 828      54.918  51.103   0.928  1.00 20.00
ATOM    100  CA  ASP A 828      54.261  52.360   1.165  1.00 20.00
ATOM    101  C   ASP A 828      54.815  53.309   2.231  1.00 20.00
ATOM    102  O   ASP A 828      55.694  52.973   3.033  1.00 20.00
ATOM    103  CB  ASP A 828      52.856  52.049   1.499  1.00 20.00
ATOM    104  CG  ASP A 828      52.783  50.948   2.460  1.00 20.00
ATOM    105  OD1 ASP A 828      52.099  49.943   2.182  1.00 20.00
ATOM    106  OD2 ASP A 828      53.439  51.088   3.504  1.00 20.00
ATOM    108  N   VAL A 829      54.278  54.522   2.216  1.00 20.00
ATOM    109  CA  VAL A 829      54.681  55.525   3.158  1.00 20.00
ATOM    110  C   VAL A 829      54.405  54.794   4.471  1.00 20.00
ATOM    111  O   VAL A 829      53.373  54.176   4.562  1.00 20.00
ATOM    112  CB  VAL A 829      53.772  56.742   2.971  1.00 20.00
ATOM    114  N   ILE A 830      55.298  54.759   5.453  1.00 20.00
ATOM    115  CA  ILE A 830      54.911  54.062   6.686  1.00 20.00
ATOM    116  C   ILE A 830      54.690  55.170   7.627  1.00 20.00
ATOM    117  O   ILE A 830      55.296  55.229   8.696  1.00 20.00
ATOM    118  CB  ILE A 830      56.004  53.170   7.366  1.00 20.00
ATOM    119  CG1 ILE A 830      56.458  52.054   6.437  1.00 20.00
ATOM    120  CG2 ILE A 830      55.435  52.493   8.636  1.00 20.00
ATOM    121  CD1 ILE A 830      57.626  51.361   6.996  1.00 20.00
ATOM    123  N   GLY A 831      53.802  56.059   7.244  1.00 20.00
ATOM    124  CA  GLY A 831      53.588  57.205   8.087  1.00 20.00
ATOM    125  C   GLY A 831      54.694  58.162   7.693  1.00 20.00
ATOM    126  O   GLY A 831      55.359  57.972   6.691  1.00 20.00
ATOM    128  N   GLU A 832      54.888  59.180   8.505  1.00 20.00
ATOM    129  CA  GLU A 832      55.889  60.205   8.260  1.00 20.00
ATOM    130  C   GLU A 832      57.146  59.876   7.452  1.00 20.00
ATOM    131  O   GLU A 832      57.220  58.893   6.667  1.00 20.00
ATOM    132  CB  GLU A 832      56.346  60.832   9.592  1.00 20.00
ATOM    133  CG  GLU A 832      56.473  62.337   9.489  1.00 20.00
ATOM    134  CD  GLU A 832      55.501  62.908   8.468  1.00 20.00
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FIG. 4B

ATOM	135	OE1	GLU	A	832	54.643	63.721	8.897	1.00	20.00
ATOM	136	OE2	GLU	A	832	55.599	62.524	7.266	1.00	20.00
ATOM	138	N	GLY	A	833	58.134	60.754	7.680	1.00	20.00
ATOM	139	CA	GLY	A	833	59.440	60.670	7.054	1.00	20.00
ATOM	140	C	GLY	A	833	60.222	61.871	7.561	1.00	20.00
ATOM	141	O	GLY	A	833	60.606	61.957	8.770	1.00	20.00
ATOM	143	N	ASN	A	834	60.380	62.816	6.621	1.00	20.00
ATOM	144	CA	ASN	A	834	61.123	64.085	6.772	1.00	20.00
ATOM	145	C	ASN	A	834	62.555	63.797	7.139	1.00	20.00
ATOM	146	O	ASN	A	834	62.796	63.133	8.141	1.00	20.00
ATOM	147	CB	ASN	A	834	60.584	65.052	7.859	1.00	20.00
ATOM	148	CG	ASN	A	834	61.664	66.125	8.258	1.00	20.00
ATOM	149	OD1	ASN	A	834	61.998	66.999	7.444	1.00	20.00
ATOM	150	ND2	ASN	A	834	62.224	66.022	9.491	1.00	20.00
ATOM	154	N	PHE	A	835	63.474	64.373	6.355	1.00	20.00
ATOM	155	CA	PHE	A	835	64.922	64.216	6.526	1.00	20.00
ATOM	156	C	PHE	A	835	64.972	63.040	7.488	1.00	20.00
ATOM	157	O	PHE	A	835	65.560	63.063	8.616	1.00	20.00
ATOM	158	CB	PHE	A	835	65.545	65.547	7.028	1.00	20.00
ATOM	159	CG	PHE	A	835	65.828	66.560	5.895	1.00	20.00
ATOM	160	CD1	PHE	A	835	65.442	67.913	6.013	1.00	20.00
ATOM	161	CD2	PHE	A	835	66.534	66.176	4.742	1.00	20.00
ATOM	162	CE1	PHE	A	835	65.761	68.870	5.004	1.00	20.00
ATOM	163	CE2	PHE	A	835	66.859	67.138	3.725	1.00	20.00
ATOM	164	CZ	PHE	A	835	66.469	68.482	3.867	1.00	20.00
ATOM	166	N	GLY	A	836	64.251	62.029	6.984	1.00	20.00
ATOM	167	CA	GLY	A	836	64.025	60.759	7.647	1.00	20.00
ATOM	168	C	GLY	A	836	62.817	60.226	6.884	1.00	20.00
ATOM	169	O	GLY	A	836	61.874	59.661	7.452	1.00	20.00
ATOM	171	N	GLN	A	837	62.827	60.432	5.571	1.00	20.00
ATOM	172	CA	GLN	A	837	61.720	59.959	4.749	1.00	20.00
ATOM	173	C	GLN	A	837	61.471	58.496	5.132	1.00	20.00
ATOM	174	O	GLN	A	837	62.278	57.647	4.742	1.00	20.00
ATOM	175	CB	GLN	A	837	62.112	60.066	3.253	1.00	20.00
ATOM	176	CG	GLN	A	837	63.459	60.807	2.984	1.00	20.00
ATOM	177	CD	GLN	A	837	63.541	61.552	1.605	1.00	20.00
ATOM	178	OE1	GLN	A	837	64.298	62.539	1.447	1.00	20.00
ATOM	179	NE2	GLN	A	837	62.786	61.053	0.607	1.00	20.00
ATOM	183	N	VAL	A	838	60.400	58.162	5.872	1.00	20.00
ATOM	184	CA	VAL	A	838	60.233	56.718	6.211	1.00	20.00
ATOM	185	C	VAL	A	838	59.296	55.833	5.400	1.00	20.00
ATOM	186	O	VAL	A	838	58.143	55.705	5.734	1.00	20.00
ATOM	187	CB	VAL	A	838	59.824	56.442	7.659	1.00	20.00
ATOM	188	CG1	VAL	A	838	60.786	55.456	8.230	1.00	20.00
ATOM	189	CG2	VAL	A	838	59.760	57.703	8.475	1.00	20.00
ATOM	191	N	LEU	A	839	59.820	55.181	4.373	1.00	20.00
ATOM	192	CA	LEU	A	839	59.031	54.306	3.542	1.00	20.00
ATOM	193	C	LEU	A	839	58.983	52.882	4.069	1.00	20.00
ATOM	194	O	LEU	A	839	59.676	52.547	5.015	1.00	20.00
ATOM	195	CB	LEU	A	839	59.566	54.385	2.111	1.00	20.00
ATOM	196	CG	LEU	A	839	58.912	55.608	1.396	1.00	20.00
ATOM	197	CD1	LEU	A	839	58.295	56.545	2.426	1.00	20.00
ATOM	198	CD2	LEU	A	839	59.886	56.367	0.533	1.00	20.00
ATOM	200	N	LYS	A	840	58.119	52.049	3.503	1.00	20.00
ATOM	201	CA	LYS	A	840	58.031	50.646	3.945	1.00	20.00
ATOM	202	C	LYS	A	840	58.687	49.724	2.927	1.00	20.00
ATOM	203	O	LYS	A	840	58.645	49.971	1.725	1.00	20.00

FIG. 4C

ATOM	204	CB	LYS	A	840	56.577	50.198	4.145	1.00 20.00
ATOM	205	CG	LYS	A	840	56.445	49.166	5.251	1.00 20.00
ATOM	206	CD	LYS	A	840	55.843	47.830	4.789	1.00 20.00
ATOM	207	CE	LYS	A	840	55.173	47.110	5.960	1.00 20.00
ATOM	208	NZ	LYS	A	840	56.154	46.444	6.801	1.00 20.00
ATOM	213	N	ALA	A	841	59.302	48.650	3.383	1.00 20.00
ATOM	214	CA	ALA	A	841	59.929	47.798	2.393	1.00 20.00
ATOM	215	C	ALA	A	841	60.199	46.360	2.787	1.00 20.00
ATOM	216	O	ALA	A	841	60.460	46.044	3.971	1.00 20.00
ATOM	217	CB	ALA	A	841	61.224	48.462	1.884	1.00 20.00
ATOM	219	N	ARG	A	842	60.111	45.506	1.759	1.00 20.00
ATOM	220	CA	ARG	A	842	60.347	44.075	1.824	1.00 20.00
ATOM	221	C	ARG	A	842	61.797	43.918	1.340	1.00 20.00
ATOM	222	O	ARG	A	842	62.105	43.967	0.158	1.00 20.00
ATOM	223	CB	ARG	A	842	59.365	43.360	0.902	1.00 20.00
ATOM	225	N	ILE	A	843	62.688	43.746	2.293	1.00 20.00
ATOM	226	CA	ILE	A	843	64.113	43.638	2.034	1.00 20.00
ATOM	227	C	ILE	A	843	64.747	42.223	2.205	1.00 20.00
ATOM	228	O	ILE	A	843	64.527	41.503	3.201	1.00 20.00
ATOM	229	CB	ILE	A	843	64.846	44.662	2.928	1.00 20.00
ATOM	230	CG1	ILE	A	843	65.867	45.411	2.103	1.00 20.00
ATOM	231	CG2	ILE	A	843	65.469	43.996	4.130	1.00 20.00
ATOM	232	CD1	ILE	A	843	66.176	44.779	0.772	1.00 20.00
ATOM	234	N	LYS	A	844	65.549	41.837	1.226	1.00 20.00
ATOM	235	CA	LYS	A	844	66.190	40.551	1.273	1.00 20.00
ATOM	236	C	LYS	A	844	67.652	40.641	1.709	1.00 20.00
ATOM	237	O	LYS	A	844	68.540	40.820	0.869	1.00 20.00
ATOM	238	CB	LYS	A	844	66.093	39.875	-0.111	1.00 20.00
ATOM	240	N	LYS	A	845	67.897	40.510	3.014	1.00 20.00
ATOM	241	CA	LYS	A	845	69.261	40.516	3.545	1.00 20.00
ATOM	242	C	LYS	A	845	69.917	39.112	3.335	1.00 20.00
ATOM	243	O	LYS	A	845	69.306	38.060	3.678	1.00 20.00
ATOM	244	CB	LYS	A	845	69.255	40.857	5.035	1.00 20.00
ATOM	246	N	ASP	A	846	71.148	39.140	2.765	1.00 20.00
ATOM	247	CA	ASP	A	846	72.022	37.977	2.481	1.00 20.00
ATOM	248	C	ASP	A	846	71.224	36.671	2.559	1.00 20.00
ATOM	249	O	ASP	A	846	71.231	35.953	3.581	1.00 20.00
ATOM	250	CB	ASP	A	846	73.214	37.987	3.484	1.00 20.00
ATOM	251	CG	ASP	A	846	74.448	37.141	3.002	1.00 20.00
ATOM	252	OD1	ASP	A	846	74.788	37.167	1.784	1.00 20.00
ATOM	253	OD2	ASP	A	846	75.078	36.450	3.869	1.00 20.00
ATOM	255	N	GLY	A	847	70.497	36.405	1.476	1.00 20.00
ATOM	256	CA''	GLY	A	847	69.670	35.206	1.405	1.00 20.00
ATOM	257	C	GLY	A	847	68.642	35.071	2.527	1.00 20.00
ATOM	258	O	GLY	A	847	68.972	34.604	3.636	1.00 20.00
ATOM	260	N	LEU	A	848	67.406	35.481	2.198	1.00 20.00
ATOM	261	CA	LEU	A	848	66.192	35.495	3.049	1.00 20.00
ATOM	262	C	LEU	A	848	65.707	36.956	3.333	1.00 20.00
ATOM	263	O	LEU	A	848	66.470	37.844	3.751	1.00 20.00
ATOM	264	CB	LEU	A	848	66.402	34.666	4.318	1.00 20.00
ATOM	265	CG	LEU	A	848	66.559	35.338	5.653	1.00 20.00
ATOM	266	CD1	LEU	A	848	66.241	34.369	6.804	1.00 20.00
ATOM	267	CD2	LEU	A	848	68.011	35.849	5.755	1.00 20.00
ATOM	269	N	ARG	A	849	64.434	37.188	3.011	1.00 20.00
ATOM	270	CA	ARG	A	849	63.793	38.491	3.149	1.00 20.00
ATOM	271	C	ARG	A	849	63.495	38.916	4.576	1.00 20.00
ATOM	272	O	ARG	A	849	63.795	38.195	5.542	1.00 20.00

FIG. 4D

ATOM	273	CB	ARG	A	849	62.465	38.508	2.388	1.00 20.00
ATOM	274	CG	ARG	A	849	62.570	38.136	0.936	1.00 20.00
ATOM	275	CD	ARG	A	849	61.348	38.648	0.182	1.00 20.00
ATOM	276	NE	ARG	A	849	61.060	37.918	-1.060	1.00 20.00
ATOM	277	CZ	ARG	A	849	60.337	36.795	-1.117	1.00 20.00
ATOM	278	NH1	ARG	A	849	59.833	36.281	0.018	1.00 20.00
ATOM	279	NH2	ARG	A	849	60.113	36.198	-2.308	1.00 20.00
ATOM	286	N	MET	A	850	62.903	40.112	4.678	1.00 20.00
ATOM	287	CA	MET	A	850	62.466	40.710	5.938	1.00 20.00
ATOM	288	C	MET	A	850	61.786	42.087	5.756	1.00 20.00
ATOM	289	O	MET	A	850	61.816	42.702	4.694	1.00 20.00
ATOM	290	CB	MET	A	850	63.628	40.814	6.953	1.00 20.00
ATOM	291	CG	MET	A	850	65.005	41.061	6.376	1.00 20.00
ATOM	292	SD	MET	A	850	66.205	41.855	7.507	1.00 20.00
ATOM	293	CE	MET	A	850	66.021	40.869	9.036	1.00 20.00
ATOM	295	N	ASP	A	851	61.105	42.523	6.800	1.00 20.00
ATOM	296	CA	ASP	A	851	60.477	43.812	6.787	1.00 20.00
ATOM	297	C	ASP	A	851	61.586	44.780	7.213	1.00 20.00
ATOM	298	O	ASP	A	851	62.559	44.403	7.904	1.00 20.00
ATOM	299	CB	ASP	A	851	59.381	43.909	7.855	1.00 20.00
ATOM	300	CG	ASP	A	851	58.154	43.076	7.546	1.00 20.00
ATOM	301	OD1	ASP	A	851	57.886	42.769	6.352	1.00 20.00
ATOM	302	OD2	ASP	A	851	57.452	42.744	8.545	1.00 20.00
ATOM	304	N	ALA	A	852	61.366	46.044	6.842	1.00 20.00
ATOM	305	CA	ALA	A	852	62.230	47.173	7.161	1.00 20.00
ATOM	306	C	ALA	A	852	61.483	48.457	6.814	1.00 20.00
ATOM	307	O	ALA	A	852	60.631	48.480	5.902	1.00 20.00
ATOM	308	CB	ALA	A	852	63.507	47.092	6.332	1.00 20.00
ATOM	310	N	ALA	A	853	61.774	49.522	7.546	1.00 20.00
ATOM	311	CA	ALA	A	853	61.205	50.818	7.189	1.00 20.00
ATOM	312	C	ALA	A	853	62.439	51.427	6.518	1.00 20.00
ATOM	313	O	ALA	A	853	63.529	50.919	6.771	1.00 20.00
ATOM	314	CB	ALA	A	853	60.812	51.581	8.418	1.00 20.00
ATOM	316	N	ILE	A	854	62.300	52.470	5.685	1.00 20.00
ATOM	317	CA	ILE	A	854	63.436	53.072	4.960	1.00 20.00
ATOM	318	C	ILE	A	854	63.501	54.570	5.142	1.00 20.00
ATOM	319	O	ILE	A	854	62.478	55.156	5.413	1.00 20.00
ATOM	320	CB	ILE	A	854	63.313	52.777	3.457	1.00 20.00
ATOM	321	CG1	ILE	A	854	63.527	51.284	3.195	1.00 20.00
ATOM	322	CG2	ILE	A	854	64.353	53.554	2.664	1.00 20.00
ATOM	323	CD1	ILE	A	854	64.906	50.722	3.717	1.00 20.00
ATOM	325	N	LYS	A	855	64.699	55.189	5.023	1.00 20.00
ATOM	326	CA	LYS	A	855	64.901	56.684	5.158	1.00 20.00
ATOM	327	C	LYS	A	855	65.800	57.286	4.079	1.00 20.00
ATOM	328	O	LYS	A	855	65.740	56.867	2.946	1.00 20.00
ATOM	329	CB	LYS	A	855	65.417	57.088	6.580	1.00 20.00
ATOM	330	CG	LYS	A	855	66.949	57.267	6.792	1.00 20.00
ATOM	331	CD	LYS	A	855	67.333	57.776	8.262	1.00 20.00
ATOM	332	CE	LYS	A	855	68.597	57.022	8.917	1.00 20.00
ATOM	333	NZ	LYS	A	855	69.828	57.804	9.506	1.00 20.00
ATOM	338	N	ARG	A	856	66.573	58.311	4.439	1.00 20.00
ATOM	339	CA	ARG	A	856	67.569	59.035	3.573	1.00 20.00
ATOM	340	C	ARG	A	856	66.957	60.199	2.856	1.00 20.00
ATOM	341	O	ARG	A	856	66.375	60.027	1.793	1.00 20.00
ATOM	342	CB	ARG	A	856	68.288	58.135	2.533	1.00 20.00
ATOM	343	CG	ARG	A	856	69.278	58.948	1.706	1.00 20.00
ATOM	344	CD	ARG	A	856	68.965	58.943	0.179	1.00 20.00

FIG. 4E

```
ATOM    345  NE  ARG A 856      68.880  60.276  -0.435  1.00 20.00
ATOM    346  CZ  ARG A 856      68.623  60.497  -1.732  1.00 20.00
ATOM    347  NH1 ARG A 856      68.425  59.484  -2.568  1.00 20.00
ATOM    348  NH2 ARG A 856      68.555  61.750  -2.204  1.00 20.00
ATOM    355  N   MET A 857      67.166  61.381   3.446  1.00 20.00
ATOM    356  CA  MET A 857      66.581  62.674   2.991  1.00 20.00
ATOM    357  C   MET A 857      67.495  63.831   2.508  1.00 20.00
ATOM    358  O   MET A 857      68.427  64.269   3.254  1.00 20.00
ATOM    359  CB  MET A 857      65.682  63.220   4.125  1.00 20.00
ATOM    360  CG  MET A 857      64.287  63.699   3.730  1.00 20.00
ATOM    361  SD  MET A 857      62.819  63.037   4.735  1.00 20.00
ATOM    362  CE  MET A 857      61.431  64.067   3.876  1.00 20.00
ATOM    363  OXT MET A 857      67.199  64.316   1.383  1.00 20.00
ATOM    365  N   ASP A 864      77.202  66.313  -0.527  1.00 20.00
ATOM    366  CA  ASP A 864      77.838  67.381  -1.394  1.00 20.00
ATOM    367  C   ASP A 864      78.591  68.418  -0.580  1.00 20.00
ATOM    368  O   ASP A 864      79.619  68.925  -1.043  1.00 20.00
ATOM    369  CB  ASP A 864      76.768  68.105  -2.272  1.00 20.00
ATOM    373  N   ASP A 865      78.090  68.727   0.620  1.00 20.00
ATOM    374  CA  ASP A 865      78.709  69.760   1.436  1.00 20.00
ATOM    375  C   ASP A 865      78.128  69.958   2.819  1.00 20.00
ATOM    376  O   ASP A 865      78.844  70.418   3.695  1.00 20.00
ATOM    377  CB  ASP A 865      78.665  71.087   0.683  1.00 20.00
ATOM    379  N   HIS A 866      76.832  69.683   3.014  1.00 20.00
ATOM    380  CA  HIS A 866      76.223  69.807   4.364  1.00 20.00
ATOM    381  C   HIS A 866      76.425  68.436   4.955  1.00 20.00
ATOM    382  O   HIS A 866      76.537  68.227   6.178  1.00 20.00
ATOM    383  CB  HIS A 866      74.699  70.145   4.303  1.00 20.00
ATOM    384  CG  HIS A 866      73.836  69.068   3.706  1.00 20.00
ATOM    385  ND1 HIS A 866      73.511  69.036   2.360  1.00 20.00
ATOM    386  CD2 HIS A 866      73.145  68.054   4.285  1.00 20.00
ATOM    387  CE1 HIS A 866      72.653  68.054   2.140  1.00 20.00
ATOM    388  NE2 HIS A 866      72.416  67.443   3.290  1.00 20.00
ATOM    392  N   ARG A 867      76.481  67.523   3.992  1.00 20.00
ATOM    393  CA  ARG A 867      76.682  66.101   4.167  1.00 20.00
ATOM    394  C   ARG A 867      77.752  65.727   5.193  1.00 20.00
ATOM    395  O   ARG A 867      78.957  65.919   4.933  1.00 20.00
ATOM    396  CB  ARG A 867      77.059  65.491   2.804  1.00 20.00
ATOM    397  CG  ARG A 867      78.073  66.314   2.001  1.00 20.00
ATOM    398  CD  ARG A 867      79.548  66.134   2.438  1.00 20.00
ATOM    399  NE  ARG A 867      80.417  67.048   1.682  1.00 20.00
ATOM    400  CZ  ARG A 867      81.270  67.924   2.231  1.00 20.00
ATOM    401  NH1 ARG A 867      81.391  68.025   3.566  1.00 20.00
ATOM    402  NH2 ARG A 867      81.977  68.729   1.428  1.00 20.00
ATOM    409  N   ASP A 868      77.304  65.205   6.345  1.00 20.00
ATOM    410  CA  ASP A 868      78.197  64.729   7.417  1.00 20.00
ATOM    411  C   ASP A 868      77.784  63.290   7.881  1.00 20.00
ATOM    412  O   ASP A 868      77.720  62.981   9.089  1.00 20.00
ATOM    413  CB  ASP A 868      78.199  65.733   8.593  1.00 20.00
ATOM    414  CG  ASP A 868      77.414  65.248   9.815  1.00 20.00
ATOM    415  OD1 ASP A 868      76.266  64.747   9.611  1.00 20.00
ATOM    416  OD2 ASP A 868      77.931  65.385  10.971  1.00 20.00
ATOM    418  N   PHE A 869      77.560  62.391   6.921  1.00 20.00
ATOM    419  CA  PHE A 869      77.119  61.033   7.261  1.00 20.00
ATOM    420  C   PHE A 869      78.080  59.895   6.841  1.00 20.00
ATOM    421  O   PHE A 869      78.526  59.819   5.663  1.00 20.00
ATOM    422  CB  PHE A 869      75.738  60.806   6.625  1.00 20.00
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FIG. 4F

ATOM	423	CG	PHE	A	869	75.685	61.221	5.199	1.00 20.00
ATOM	424	CD1	PHE	A	869	75.561	62.560	4.861	1.00 20.00
ATOM	425	CD2	PHE	A	869	75.848	60.286	4.190	1.00 20.00
ATOM	426	CE1	PHE	A	869	75.612	62.955	3.509	1.00 20.00
ATOM	427	CE2	PHE	A	869	75.896	60.680	2.838	1.00 20.00
ATOM	428	CZ	PHE	A	869	75.779	62.022	2.496	1.00 20.00
ATOM	430	N	ALA	A	870	78.350	59.018	7.812	1.00 20.00
ATOM	431	CA	ALA	A	870	79.231	57.831	7.715	1.00 20.00
ATOM	432	C	ALA	A	870	79.352	57.560	9.172	1.00 20.00
ATOM	433	O	ALA	A	870	78.350	57.359	9.840	1.00 20.00
ATOM	434	CB	ALA	A	870	80.624	58.132	7.160	1.00 20.00
ATOM	436	N	GLY	A	871	80.558	57.601	9.698	1.00 20.00
ATOM	437	CA	GLY	A	871	80.674	57.344	11.112	1.00 20.00
ATOM	438	C	GLY	A	871	79.343	57.592	11.791	1.00 20.00
ATOM	439	O	GLY	A	871	78.672	56.648	12.170	1.00 20.00
ATOM	441	N	GLU	A	872	78.958	58.864	11.901	1.00 20.00
ATOM	442	CA	GLU	A	872	77.690	59.258	12.529	1.00 20.00
ATOM	443	C	GLU	A	872	76.698	58.115	12.297	1.00 20.00
ATOM	444	O	GLU	A	872	76.096	57.579	13.241	1.00 20.00
ATOM	445	CB	GLU	A	872	77.178	60.602	11.939	1.00 20.00
ATOM	446	CG	GLU	A	872	76.581	60.552	10.530	1.00 20.00
ATOM	447	CD	GLU	A	872	75.027	60.750	10.507	1.00 20.00
ATOM	448	OE1	GLU	A	872	74.433	60.770	9.383	1.00 20.00
ATOM	449	OE2	GLU	A	872	74.405	60.881	11.596	1.00 20.00
ATOM	451	N	LEU	A	873	76.545	57.753	11.028	1.00 20.00
ATOM	452	CA	LEU	A	873	75.726	56.633	10.649	1.00 20.00
ATOM	453	C	LEU	A	873	76.593	55.505	11.273	1.00 20.00
ATOM	454	O	LEU	A	873	76.715	55.463	12.500	1.00 20.00
ATOM	455	CB	LEU	A	873	75.658	56.527	9.101	1.00 20.00
ATOM	457	N	GLU	A	874	77.195	54.620	10.458	1.00 20.00
ATOM	458	CA	GLU	A	874	78.069	53.539	10.975	1.00 20.00
ATOM	459	C	GLU	A	874	77.903	53.535	12.468	1.00 20.00
ATOM	460	O	GLU	A	874	76.948	52.968	12.998	1.00 20.00
ATOM	461	CB	GLU	A	874	79.526	53.831	10.639	1.00 20.00
ATOM	463	N	VAL	A	875	78.838	54.222	13.116	1.00 20.00
ATOM	464	CA	VAL	A	875	78.847	54.419	14.567	1.00 20.00
ATOM	465	C	VAL	A	875	77.770	53.658	15.342	1.00 20.00
ATOM	466	O	VAL	A	875	78.065	52.892	16.266	1.00 20.00
ATOM	467	CB	VAL	A	875	78.756	55.961	14.897	1.00 20.00
ATOM	469	N	LEU	A	876	76.520	53.887	14.966	1.00 20.00
ATOM	470	CA	LEU	A	876	75.408	53.237	15.630	1.00 20.00
ATOM	471	C	LEU	A	876	75.957	51.873	16.004	1.00 20.00
ATOM	472	O	LEU	A	876	75.727	51.387	17.126	1.00 20.00
ATOM	473	CB	LEU	A	876	74.208	53.192	14.684	1.00 20.00
ATOM	474	CG	LEU	A	876	73.839	54.662	14.399	1.00 20.00
ATOM	475	CD1	LEU	A	876	73.193	54.792	13.056	1.00 20.00
ATOM	476	CD2	LEU	A	876	72.942	55.198	15.481	1.00 20.00
ATOM	478	N	CYS	A	877	76.744	51.320	15.071	1.00 20.00
ATOM	479	CA	CYS	A	877	77.459	50.027	15.212	1.00 20.00
ATOM	480	C	CYS	A	877	77.658	49.645	16.685	1.00 20.00
ATOM	481	O	CYS	A	877	77.099	48.656	17.205	1.00 20.00
ATOM	482	CB	CYS	A	877	78.855	50.137	14.546	1.00 20.00
ATOM	483	SG	CYS	A	877	79.630	51.894	14.438	1.00 20.00
ATOM	485	N	LYS	A	878	78.447	50.496	17.337	1.00 20.00
ATOM	486	CA	LYS	A	878	78.789	50.363	18.762	1.00 20.00
ATOM	487	C	LYS	A	878	77.629	49.811	19.612	1.00 20.00
ATOM	488	O	LYS	A	878	77.847	49.438	20.805	1.00 20.00

FIG. 4G

ATOM	489	CB	LYS	A	878	79.260	51.733	19.351	1.00 20.00
ATOM	490	CG	LYS	A	878	80.718	52.114	19.017	1.00 20.00
ATOM	491	CD	LYS	A	878	81.321	52.986	20.114	1.00 20.00
ATOM	492	CE	LYS	A	878	81.612	54.418	19.609	1.00 20.00
ATOM	493	NZ	LYS	A	878	81.754	54.601	18.098	1.00 20.00
ATOM	498	N	LEU	A	879	76.427	49.792	19.000	1.00 20.00
ATOM	499	CA	LEU	A	879	75.203	49.320	19.634	1.00 20.00
ATOM	500	C	LEU	A	879	74.179	49.039	18.584	1.00 20.00
ATOM	501	O	LEU	A	879	73.068	49.544	18.652	1.00 20.00
ATOM	502	CB	LEU	A	879	74.620	50.336	20.651	1.00 20.00
ATOM	503	CG	LEU	A	879	74.799	51.863	20.603	1.00 20.00
ATOM	504	CD1	LEU	A	879	75.966	52.280	21.461	1.00 20.00
ATOM	505	CD2	LEU	A	879	75.015	52.321	19.200	1.00 20.00
ATOM	507	N	GLY	A	880	74.546	48.227	17.597	1.00 20.00
ATOM	508	CA	GLY	A	880	73.551	47.899	16.578	1.00 20.00
ATOM	509	C	GLY	A	880	72.345	47.314	17.330	1.00 20.00
ATOM	510	O	GLY	A	880	71.296	47.906	17.464	1.00 20.00
ATOM	512	N	HIS	A	881	72.545	46.101	17.820	1.00 20.00
ATOM	513	CA	HIS	A	881	71.575	45.353	18.572	1.00 20.00
ATOM	514	C	HIS	A	881	71.402	46.024	19.917	1.00 20.00
ATOM	515	O	HIS	A	881	71.758	47.183	20.106	1.00 20.00
ATOM	516	CB	HIS	A	881	72.059	43.906	18.744	1.00 20.00
ATOM	517	CG	HIS	A	881	71.015	42.958	19.255	1.00 20.00
ATOM	518	ND1	HIS	A	881	69.952	42.520	18.485	1.00 20.00
ATOM	519	CD2	HIS	A	881	70.877	42.349	20.464	1.00 20.00
ATOM	520	CE1	HIS	A	881	69.207	41.691	19.197	1.00 20.00
ATOM	521	NE2	HIS	A	881	69.746	41.566	20.402	1.00 20.00
ATOM	525	N	HIS	A	882	70.870	45.217	20.817	1.00 20.00
ATOM	526	CA	HIS	A	882	70.420	45.429	22.177	1.00 20.00
ATOM	527	C	HIS	A	882	68.935	45.241	21.763	1.00 20.00
ATOM	528	O	HIS	A	882	68.440	45.758	20.724	1.00 20.00
ATOM	529	CB	HIS	A	882	70.704	46.804	22.806	1.00 20.00
ATOM	530	CG	HIS	A	882	70.491	46.812	24.295	1.00 20.00
ATOM	531	ND1	HIS	A	882	69.252	46.654	24.868	1.00 20.00
ATOM	532	CD2	HIS	A	882	71.365	46.839	25.325	1.00 20.00
ATOM	533	CE1	HIS	A	882	69.373	46.579	26.183	1.00 20.00
ATOM	534	NE2	HIS	A	882	70.645	46.686	26.486	1.00 20.00
ATOM	538	N	PRO	A	883	68.210	44.463	22.547	1.00 20.00
ATOM	539	CA	PRO	A	883	66.820	44.253	22.152	1.00 20.00
ATOM	540	C	PRO	A	883	66.019	45.510	22.212	1.00 20.00
ATOM	541	O	PRO	A	883	65.100	45.685	21.439	1.00 20.00
ATOM	542	CB	PRO	A	883	66.309	43.176	23.108	1.00 20.00
ATOM	543	@G	PRO	A	883	67.285	43.129	24.211	1.00 20.00
ATOM	544	CD	PRO	A	883	68.560	43.829	23.819	1.00 20.00
ATOM	545	N	ASN	A	884	66.414	46.408	23.098	1.00 20.00
ATOM	546	CA	ASN	A	884	65.710	47.650	23.263	1.00 20.00
ATOM	547	C	ASN	A	884	66.169	48.856	22.439	1.00 20.00
ATOM	548	O	ASN	A	884	65.801	49.977	22.723	1.00 20.00
ATOM	549	CB	ASN	A	884	65.672	47.898	24.749	1.00 20.00
ATOM	550	CG	ASN	A	884	65.444	46.594	25.498	1.00 20.00
ATOM	551	OD1	ASN	A	884	65.835	46.388	26.649	1.00 20.00
ATOM	552	ND2	ASN	A	884	64.817	45.687	24.802	1.00 20.00
ATOM	556	N	ILE	A	885	66.917	48.603	21.375	1.00 20.00
ATOM	557	CA	ILE	A	885	67.391	49.655	20.482	1.00 20.00
ATOM	558	C	ILE	A	885	67.205	49.202	19.020	1.00 20.00
ATOM	559	O	ILE	A	885	67.847	48.251	18.589	1.00 20.00
ATOM	560	CB	ILE	A	885	68.930	50.021	20.761	1.00 20.00

FIG. 4H

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ATOM    561  CG1 ILE A 885      69.032  50.962  21.954  1.00 20.00
ATOM    562  CG2 ILE A 885      69.529  50.830  19.639  1.00 20.00
ATOM    563  CD1 ILE A 885      70.397  51.213  22.385  1.00 20.00
ATOM    565  N   ILE A 886      66.325  49.886  18.282  1.00 20.00
ATOM    566  CA  ILE A 886      66.030  49.608  16.871  1.00 20.00
ATOM    567  C   ILE A 886      67.338  49.271  16.206  1.00 20.00
ATOM    568  O   ILE A 886      68.363  49.491  16.788  1.00 20.00
ATOM    569  CB  ILE A 886      65.331  50.854  16.183  1.00 20.00
ATOM    570  CG1 ILE A 886      63.806  50.758  16.349  1.00 20.00
ATOM    571  CG2 ILE A 886      65.568  50.868  14.691  1.00 20.00
ATOM    572  CD1 ILE A 886      63.134  49.624  15.492  1.00 20.00
ATOM    574  N   ASN A 887      67.347  48.757  14.990  1.00 20.00
ATOM    575  CA  ASN A 887      68.628  48.381  14.442  1.00 20.00
ATOM    576  C   ASN A 887      68.846  48.692  13.013  1.00 20.00
ATOM    577  O   ASN A 887      67.889  48.902  12.273  1.00 20.00
ATOM    578  CB  ASN A 887      68.827  46.892  14.597  1.00 20.00
ATOM    579  CG  ASN A 887      70.276  46.512  14.731  1.00 20.00
ATOM    580  OD1 ASN A 887      71.015  46.382  13.725  1.00 20.00
ATOM    581  ND2 ASN A 887      70.702  46.315  15.979  1.00 20.00
ATOM    585  N   LEU A 888      70.118  48.684  12.604  1.00 20.00
ATOM    586  CA  LEU A 888      70.417  48.950  11.203  1.00 20.00
ATOM    587  C   LEU A 888      70.410  47.641  10.469  1.00 20.00
ATOM    588  O   LEU A 888      71.128  46.705  10.852  1.00 20.00
ATOM    589  CB  LEU A 888      71.799  49.586  11.000  1.00 20.00
ATOM    590  CG  LEU A 888      72.125  49.333   9.517  1.00 20.00
ATOM    591  CD1 LEU A 888      71.290  50.292   8.712  1.00 20.00
ATOM    592  CD2 LEU A 888      73.594  49.451   9.207  1.00 20.00
ATOM    594  N   LEU A 889      69.617  47.531   9.425  1.00 20.00
ATOM    595  CA  LEU A 889      69.676  46.284   8.712  1.00 20.00
ATOM    596  C   LEU A 889      70.630  46.494   7.567  1.00 20.00
ATOM    597  O   LEU A 889      71.830  46.369   7.746  1.00 20.00
ATOM    598  CB  LEU A 889      68.310  45.906   8.247  1.00 20.00
ATOM    599  CG  LEU A 889      67.451  45.554   9.465  1.00 20.00
ATOM    600  CD1 LEU A 889      66.321  44.719   8.913  1.00 20.00
ATOM    601  CD2 LEU A 889      68.201  44.811  10.568  1.00 20.00
ATOM    603  N   GLY A 890      70.114  46.838   6.396  1.00 20.00
ATOM    604  CA  GLY A 890      70.971  47.127   5.254  1.00 20.00
ATOM    605  C   GLY A 890      71.310  48.613   5.048  1.00 20.00
ATOM    606  O   GLY A 890      71.237  49.441   5.951  1.00 20.00
ATOM    608  N   ALA A 891      71.684  48.930   3.819  1.00 20.00
ATOM    609  CA  ALA A 891      72.084  50.262   3.393  1.00 20.00
ATOM    610  C   ALA A 891      72.437  50.082   1.907  1.00 20.00
ATOM    611  O   ALA A 891      72.299  48.965   1.361  1.00 20.00
ATOM    612  CB  ALA A 891      73.296  50.706   4.166  1.00 20.00
ATOM    614  N   CYS A 892      72.908  51.153   1.262  1.00 20.00
ATOM    615  CA  CYS A 892      73.258  51.085  -0.166  1.00 20.00
ATOM    616  C   CYS A 892      73.174  52.468  -0.776  1.00 20.00
ATOM    617  O   CYS A 892      72.263  53.232  -0.453  1.00 20.00
ATOM    618  CB  CYS A 892      72.277  50.171  -0.952  1.00 20.00
ATOM    619  SG  CYS A 892      72.953  48.465  -1.345  1.00 20.00
ATOM    621  N   GLU A 893      74.089  52.785  -1.680  1.00 20.00
ATOM    622  CA  GLU A 893      74.062  54.101  -2.298  1.00 20.00
ATOM    623  C   GLU A 893      73.386  54.004  -3.637  1.00 20.00
ATOM    624  O   GLU A 893      73.956  53.509  -4.616  1.00 20.00
ATOM    625  CB  GLU A 893      75.483  54.655  -2.463  1.00 20.00
ATOM    626  CG  GLU A 893      76.613  53.751  -1.900  1.00 20.00
ATOM    627  CD  GLU A 893      77.227  52.860  -2.966  1.00 20.00
```

FIG. 4I

ATOM	628	OE1	GLU	A	893	76.831	52.998	-4.151	1.00 20.00
ATOM	629	OE2	GLU	A	893	78.105	52.033	-2.612	1.00 20.00
ATOM	631	N	HIS	A	894	72.140	54.427	-3.684	1.00 20.00
ATOM	632	CA	HIS	A	894	71.437	54.382	-4.949	1.00 20.00
ATOM	633	C	HIS	A	894	71.690	55.786	-5.419	1.00 20.00
ATOM	634	O	HIS	A	894	71.305	56.755	-4.750	1.00 20.00
ATOM	635	CB	HIS	A	894	69.937	54.149	-4.753	1.00 20.00
ATOM	636	CG	HIS	A	894	69.133	54.328	-6.003	1.00 20.00
ATOM	637	ND1	HIS	A	894	67.767	54.494	-5.990	1.00 20.00
ATOM	638	CD2	HIS	A	894	69.510	54.413	-7.301	1.00 20.00
ATOM	639	CE1	HIS	A	894	67.332	54.680	-7.223	1.00 20.00
ATOM	640	NE2	HIS	A	894	68.369	54.634	-8.037	1.00 20.00
ATOM	644	N	ARG	A	895	72.366	55.873	-6.556	1.00 20.00
ATOM	645	CA	ARG	A	895	72.768	57.132	-7.151	1.00 20.00
ATOM	646	C	ARG	A	895	71.873	58.311	-6.767	1.00 20.00
ATOM	647	O	ARG	A	895	70.654	58.317	-7.001	1.00 20.00
ATOM	648	CB	ARG	A	895	72.910	56.904	-8.643	1.00 20.00
ATOM	649	CG	ARG	A	895	73.918	55.775	-8.856	1.00 20.00
ATOM	650	CD	ARG	A	895	73.482	54.825	-9.910	1.00 20.00
ATOM	651	NE	ARG	A	895	74.001	55.309	-11.176	1.00 20.00
ATOM	652	CZ	ARG	A	895	73.609	54.881	-12.370	1.00 20.00
ATOM	653	NH1	ARG	A	895	72.657	53.926	-12.469	1.00 20.00
ATOM	654	NH2	ARG	A	895	74.183	55.416	-13.460	1.00 20.00
ATOM	661	N	GLY	A	896	72.510	59.315	-6.177	1.00 20.00
ATOM	662	CA	GLY	A	896	71.781	60.441	-5.654	1.00 20.00
ATOM	663	C	GLY	A	896	71.963	60.040	-4.207	1.00 20.00
ATOM	664	O	GLY	A	896	72.194	58.860	-3.967	1.00 20.00
ATOM	666	N	TYR	A	897	71.919	60.962	-3.254	1.00 20.00
ATOM	667	CA	TYR	A	897	72.066	60.604	-1.839	1.00 20.00
ATOM	668	C	TYR	A	897	71.643	59.133	-1.531	1.00 20.00
ATOM	669	O	TYR	A	897	70.959	58.507	-2.336	1.00 20.00
ATOM	670	CB	TYR	A	897	71.195	61.548	-1.039	1.00 20.00
ATOM	671	CG	TYR	A	897	71.828	62.224	0.128	1.00 20.00
ATOM	672	CD1	TYR	A	897	73.097	62.810	0.030	1.00 20.00
ATOM	673	CD2	TYR	A	897	71.116	62.358	1.321	1.00 20.00
ATOM	674	CE1	TYR	A	897	73.638	63.526	1.108	1.00 20.00
ATOM	675	CE2	TYR	A	897	71.641	63.069	2.402	1.00 20.00
ATOM	676	CZ	TYR	A	897	72.894	63.650	2.290	1.00 20.00
ATOM	677	OH	TYR	A	897	73.381	64.361	3.369	1.00 20.00
ATOM	680	N	LEU	A	898	72.001	58.564	-0.369	1.00 20.00
ATOM	681	CA	LEU	A	898	71.571	57.163	-0.196	1.00 20.00
ATOM	682	C	LEU	A	898	71.131	56.437	1.099	1.00 20.00
ATOM	683	O	LEU	A	898	71.759	56.483	2.161	1.00 20.00
ATOM	684	CB	LEU	A	898	72.542	56.240	-0.990	1.00 20.00
ATOM	686	N	TYR	A	899	70.041	55.704	0.830	1.00 20.00
ATOM	687	CA	TYR	A	899	69.162	54.833	1.624	1.00 20.00
ATOM	688	C	TYR	A	899	69.544	53.804	2.665	1.00 20.00
ATOM	689	O	TYR	A	899	70.411	52.969	2.445	1.00 20.00
ATOM	690	CB	TYR	A	899	68.268	54.076	0.657	1.00 20.00
ATOM	691	CG	TYR	A	899	67.523	54.943	-0.339	1.00 20.00
ATOM	692	CD1	TYR	A	899	68.208	55.776	-1.209	1.00 20.00
ATOM	693	CD2	TYR	A	899	66.163	54.790	-0.522	1.00 20.00
ATOM	694	CE1	TYR	A	899	67.574	56.407	-2.238	1.00 20.00
ATOM	695	CE2	TYR	A	899	65.514	55.429	-1.564	1.00 20.00
ATOM	696	CZ	TYR	A	899	66.225	56.235	-2.431	1.00 20.00
ATOM	697	OH	TYR	A	899	65.602	56.841	-3.510	1.00 20.00
ATOM	700	N	LEU	A	900	68.814	53.814	3.775	1.00 20.00

FIG. 4J

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ATOM    701  CA  LEU A 900      69.047  52.841   4.845  1.00 20.00
ATOM    702  C   LEU A 900      67.805  51.988   5.149  1.00 20.00
ATOM    703  O   LEU A 900      66.645  52.459   5.109  1.00 20.00
ATOM    704  CB  LEU A 900      69.455  53.522   6.147  1.00 20.00
ATOM    705  CG  LEU A 900      70.810  54.184   6.259  1.00 20.00
ATOM    706  CD1 LEU A 900      71.404  54.368   4.864  1.00 20.00
ATOM    707  CD2 LEU A 900      70.624  55.498   7.033  1.00 20.00
ATOM    709  N   ALA A 901      68.083  50.739   5.495  1.00 20.00
ATOM    710  CA  ALA A 901      67.043  49.813   5.811  1.00 20.00
ATOM    711  C   ALA A 901      67.113  49.495   7.275  1.00 20.00
ATOM    712  O   ALA A 901      67.828  48.577   7.670  1.00 20.00
ATOM    713  CB  ALA A 901      67.221  48.564   5.003  1.00 20.00
ATOM    715  N   ILE A 902      66.372  50.260   8.078  1.00 20.00
ATOM    716  CA  ILE A 902      66.310  50.058   9.513  1.00 20.00
ATOM    717  C   ILE A 902      65.367  48.888   9.812  1.00 20.00
ATOM    718  O   ILE A 902      64.702  48.383   8.917  1.00 20.00
ATOM    719  CB  ILE A 902      65.801  51.315  10.167  1.00 20.00
ATOM    720  CG1 ILE A 902      66.882  52.398  10.058  1.00 20.00
ATOM    721  CG2 ILE A 902      65.308  51.006  11.556  1.00 20.00
ATOM    722  CD1 ILE A 902      67.878  52.583  11.280  1.00 20.00
ATOM    724  N   GLU A 903      65.322  48.439  11.057  1.00 20.00
ATOM    725  CA  GLU A 903      64.435  47.350  11.465  1.00 20.00
ATOM    726  C   GLU A 903      62.997  47.870  11.692  1.00 20.00
ATOM    727  O   GLU A 903      62.713  48.559  12.662  1.00 20.00
ATOM    728  CB  GLU A 903      64.973  46.703  12.746  1.00 20.00
ATOM    729  CG  GLU A 903      63.985  45.965  13.580  1.00 20.00
ATOM    730  CD  GLU A 903      64.471  45.766  15.006  1.00 20.00
ATOM    731  OE1 GLU A 903      63.971  44.875  15.725  1.00 20.00
ATOM    732  OE2 GLU A 903      65.365  46.509  15.425  1.00 20.00
ATOM    734  N   TYR A 904      62.115  47.514  10.767  1.00 20.00
ATOM    735  CA  TYR A 904      60.707  47.846  10.758  1.00 20.00
ATOM    736  C   TYR A 904      59.985  47.328  11.989  1.00 20.00
ATOM    737  O   TYR A 904      60.054  46.149  12.240  1.00 20.00
ATOM    738  CB  TYR A 904      60.078  47.204   9.521  1.00 20.00
ATOM    739  CG  TYR A 904      58.553  47.146   9.537  1.00 20.00
ATOM    740  CD1 TYR A 904      57.795  48.150   8.920  1.00 20.00
ATOM    741  CD2 TYR A 904      57.868  46.125  10.188  1.00 20.00
ATOM    742  CE1 TYR A 904      56.420  48.136   8.955  1.00 20.00
ATOM    743  CE2 TYR A 904      56.498  46.115  10.223  1.00 20.00
ATOM    744  CZ  TYR A 904      55.779  47.128   9.602  1.00 20.00
ATOM    745  OH  TYR A 904      54.405  47.149   9.622  1.00 20.00
ATOM    748  N   ALA A 905      59.270  48.183  12.727  1.00 20.00
ATOM    749  CA  ALA A 905      58.503  47.772  13.931  1.00 20.00
ATOM    750  C   ALA A 905      56.987  47.506  13.620  1.00 20.00
ATOM    751  O   ALA A 905      56.395  48.128  12.744  1.00 20.00
ATOM    752  CB  ALA A 905      58.649  48.816  14.976  1.00 20.00
ATOM    754  N   PRO A 906      56.341  46.572  14.317  1.00 20.00
ATOM    755  CA  PRO A 906      54.949  46.394  13.918  1.00 20.00
ATOM    756  C   PRO A 906      53.803  46.643  14.902  1.00 20.00
ATOM    757  O   PRO A 906      52.992  45.748  15.150  1.00 20.00
ATOM    758  CB  PRO A 906      54.958  44.937  13.468  1.00 20.00
ATOM    759  CG  PRO A 906      55.981  44.280  14.584  1.00 20.00
ATOM    760  CD  PRO A 906      56.719  45.482  15.227  1.00 20.00
ATOM    761  N   HIS A 907      53.729  47.841  15.450  1.00 20.00
ATOM    762  CA  HIS A 907      52.655  48.251  16.349  1.00 20.00
ATOM    763  C   HIS A 907      52.966  49.700  16.468  1.00 20.00
ATOM    764  O   HIS A 907      52.865  50.262  17.534  1.00 20.00
```

FIG. 4K

ATOM	765	CB	HIS	A	907	52.745	47.577	17.714	1.00	20.00
ATOM	766	CG	HIS	A	907	52.656	46.090	17.650	1.00	20.00
ATOM	767	ND1	HIS	A	907	53.753	45.272	17.799	1.00	20.00
ATOM	768	CD2	HIS	A	907	51.622	45.274	17.350	1.00	20.00
ATOM	769	CE1	HIS	A	907	53.404	44.018	17.593	1.00	20.00
ATOM	770	NE2	HIS	A	907	52.116	43.993	17.318	1.00	20.00
ATOM	774	N	GLY	A	908	53.411	50.280	15.365	1.00	20.00
ATOM	775	CA	GLY	A	908	53.733	51.676	15.348	1.00	20.00
ATOM	776	C	GLY	A	908	54.622	52.111	16.486	1.00	20.00
ATOM	777	O	GLY	A	908	55.525	51.381	16.887	1.00	20.00
ATOM	779	N	ASN	A	909	54.338	53.284	17.054	1.00	20.00
ATOM	780	CA	ASN	A	909	55.183	53.854	18.094	1.00	20.00
ATOM	781	C	ASN	A	909	54.590	53.912	19.463	1.00	20.00
ATOM	782	O	ASN	A	909	53.409	54.064	19.616	1.00	20.00
ATOM	783	CB	ASN	A	909	55.545	55.270	17.672	1.00	20.00
ATOM	784	CG	ASN	A	909	54.346	56.201	17.669	1.00	20.00
ATOM	785	OD1	ASN	A	909	54.409	57.315	17.192	1.00	20.00
ATOM	786	ND2	ASN	A	909	53.260	55.738	18.210	1.00	20.00
ATOM	790	N	LEU	A	910	55.414	53.878	20.482	1.00	20.00
ATOM	791	CA	LEU	A	910	54.872	53.913	21.808	1.00	20.00
ATOM	792	C	LEU	A	910	53.703	54.890	21.927	1.00	20.00
ATOM	793	O	LEU	A	910	52.760	54.647	22.669	1.00	20.00
ATOM	794	CB	LEU	A	910	55.949	54.257	22.797	1.00	20.00
ATOM	795	CG	LEU	A	910	55.456	54.079	24.220	1.00	20.00
ATOM	796	CD1	LEU	A	910	54.921	52.676	24.488	1.00	20.00
ATOM	797	CD2	LEU	A	910	56.617	54.427	25.133	1.00	20.00
ATOM	799	N	LEU	A	911	53.725	56.005	21.219	1.00	20.00
ATOM	800	CA	LEU	A	911	52.578	56.862	21.381	1.00	20.00
ATOM	801	C	LEU	A	911	51.408	56.200	20.656	1.00	20.00
ATOM	802	O	LEU	A	911	50.700	55.442	21.275	1.00	20.00
ATOM	803	CB	LEU	A	911	52.820	58.302	20.863	1.00	20.00
ATOM	804	CG	LEU	A	911	51.958	59.498	21.354	1.00	20.00
ATOM	805	CD1	LEU	A	911	51.738	59.517	22.855	1.00	20.00
ATOM	806	CD2	LEU	A	911	52.645	60.737	20.917	1.00	20.00
ATOM	808	N	ASP	A	912	51.219	56.459	19.371	1.00	20.00
ATOM	809	CA	ASP	A	912	50.117	55.895	18.642	1.00	20.00
ATOM	810	C	ASP	A	912	49.646	54.540	19.121	1.00	20.00
ATOM	811	O	ASP	A	912	48.468	54.225	19.083	1.00	20.00
ATOM	812	CB	ASP	A	912	50.461	55.849	17.181	1.00	20.00
ATOM	813	CG	ASP	A	912	50.214	57.151	16.498	1.00	20.00
ATOM	814	OD1	ASP	A	912	50.507	57.259	15.304	1.00	20.00
ATOM	815	OD2	ASP	A	912	49.725	58.089	17.141	1.00	20.00
ATOM	817	N	PHE	A	913	50.572	53.703	19.562	1.00	20.00
ATOM	818	CA	PHE	A	913	50.168	52.405	20.098	1.00	20.00
ATOM	819	C	PHE	A	913	49.397	52.903	21.287	1.00	20.00
ATOM	820	O	PHE	A	913	48.236	53.231	21.164	1.00	20.00
ATOM	821	CB	PHE	A	913	51.355	51.585	20.547	1.00	20.00
ATOM	822	CG	PHE	A	913	51.010	50.182	20.847	1.00	20.00
ATOM	823	CD1	PHE	A	913	50.511	49.365	19.866	1.00	20.00
ATOM	824	CD2	PHE	A	913	51.133	49.688	22.122	1.00	20.00
ATOM	825	CE1	PHE	A	913	50.141	48.088	20.152	1.00	20.00
ATOM	826	CE2	PHE	A	913	50.760	48.418	22.407	1.00	20.00
ATOM	827	CZ	PHE	A	913	50.263	47.619	21.418	1.00	20.00
ATOM	829	N	LEU	A	914	50.059	53.031	22.416	1.00	20.00
ATOM	830	CA	LEU	A	914	49.400	53.584	23.572	1.00	20.00
ATOM	831	C	LEU	A	914	48.080	54.304	23.288	1.00	20.00
ATOM	832	O	LEU	A	914	47.102	54.093	23.985	1.00	20.00

FIG. 4L

ATOM	833	CB	LEU	A	914	50.342	54.549	24.244	1.00 20.00
ATOM	834	CG	LEU	A	914	51.146	53.995	25.410	1.00 20.00
ATOM	835	CD1	LEU	A	914	52.130	55.080	25.953	1.00 20.00
ATOM	836	CD2	LEU	A	914	50.142	53.501	26.466	1.00 20.00
ATOM	838	N	ARG	A	915	48.006	55.139	22.265	1.00 20.00
ATOM	839	CA	ARG	A	915	46.736	55.841	22.041	1.00 20.00
ATOM	840	C	ARG	A	915	45.650	54.970	21.526	1.00 20.00
ATOM	841	O	ARG	A	915	44.569	54.984	22.054	1.00 20.00
ATOM	842	CB	ARG	A	915	46.896	57.078	21.141	1.00 20.00
ATOM	843	CG	ARG	A	915	46.687	58.379	21.885	1.00 20.00
ATOM	844	CD	ARG	A	915	47.528	59.415	21.256	1.00 20.00
ATOM	845	NE	ARG	A	915	48.215	60.347	22.169	1.00 20.00
ATOM	846	CZ	ARG	A	915	48.763	61.482	21.760	1.00 20.00
ATOM	847	NH1	ARG	A	915	48.709	61.835	20.494	1.00 20.00
ATOM	848	NH2	ARG	A	915	49.383	62.240	22.602	1.00 20.00
ATOM	855	N	LYS	A	916	45.943	54.219	20.485	1.00 20.00
ATOM	856	CA	LYS	A	916	45.019	53.242	19.890	1.00 20.00
ATOM	857	C	LYS	A	916	44.681	52.169	20.920	1.00 20.00
ATOM	858	O	LYS	A	916	44.275	51.109	20.561	1.00 20.00
ATOM	859	CB	LYS	A	916	45.714	52.563	18.676	1.00 20.00
ATOM	860	CG	LYS	A	916	45.988	51.000	18.704	1.00 20.00
ATOM	861	CD	LYS	A	916	46.802	50.408	19.888	1.00 20.00
ATOM	862	CE	LYS	A	916	46.861	48.841	19.822	1.00 20.00
ATOM	863	NZ	LYS	A	916	46.225	47.974	20.937	1.00 20.00
ATOM	868	N	SER	A	917	44.851	52.438	22.196	1.00 20.00
ATOM	869	CA	SER	A	917	44.597	51.466	23.204	1.00 20.00
ATOM	870	C	SER	A	917	43.641	52.011	24.233	1.00 20.00
ATOM	871	O	SER	A	917	43.501	51.444	25.330	1.00 20.00
ATOM	872	CB	SER	A	917	45.891	51.147	23.883	1.00 20.00
ATOM	873	OG	SER	A	917	45.843	51.568	25.227	1.00 20.00
ATOM	876	N	ARG	A	918	43.014	53.138	23.902	1.00 20.00
ATOM	877	CA	ARG	A	918	42.041	53.822	24.775	1.00 20.00
ATOM	878	C	ARG	A	918	40.816	53.359	24.014	1.00 20.00
ATOM	879	O	ARG	A	918	40.523	53.883	22.951	1.00 20.00
ATOM	880	CB	ARG	A	918	42.260	55.365	24.669	1.00 20.00
ATOM	881	CG	ARG	A	918	43.138	56.036	25.794	1.00 20.00
ATOM	882	CD	ARG	A	918	43.547	57.502	25.488	1.00 20.00
ATOM	883	NE	ARG	A	918	44.494	57.982	26.502	1.00 20.00
ATOM	884	CZ	ARG	A	918	44.777	59.260	26.795	1.00 20.00
ATOM	885	NH1	ARG	A	918	44.211	60.289	26.165	1.00 20.00
ATOM	886	NH2	ARG	A	918	45.625	59.523	27.777	1.00 20.00
ATOM	893	N	VAL	A	919	40.135	52.333	24.507	1.00 20.00
ATOM	894	CA	VAL	A	919	39.009	51.770	23.757	1.00 20.00
ATOM	895	C	VAL	A	919	37.733	52.382	24.202	1.00 20.00
ATOM	896	O	VAL	A	919	36.750	52.427	23.450	1.00 20.00
ATOM	897	CB	VAL	A	919	38.925	50.198	23.861	1.00 20.00
ATOM	898	CG1	VAL	A	919	40.218	49.603	23.459	1.00 20.00
ATOM	899	CG2	VAL	A	919	38.550	49.746	25.275	1.00 20.00
ATOM	901	N	LEU	A	920	37.736	52.861	25.432	1.00 20.00
ATOM	902	CA	LEU	A	920	36.569	53.542	25.895	1.00 20.00
ATOM	903	C	LEU	A	920	36.303	54.630	24.864	1.00 20.00
ATOM	904	O	LEU	A	920	35.276	55.259	24.906	1.00 20.00
ATOM	905	CB	LEU	A	920	36.815	54.146	27.236	1.00 20.00
ATOM	906	CG	LEU	A	920	35.641	54.652	28.011	1.00 20.00
ATOM	907	CD1	LEU	A	920	35.060	53.567	28.831	1.00 20.00
ATOM	908	CD2	LEU	A	920	36.155	55.768	28.901	1.00 20.00
ATOM	910	N	GLU	A	921	37.224	54.824	23.926	1.00 20.00

FIG. 4M

ATOM	911	CA	GLU	A	921	37.081	55.783	22.850	1.00 20.00
ATOM	912	C	GLU	A	921	37.413	55.109	21.541	1.00 20.00
ATOM	913	O	GLU	A	921	37.205	55.677	20.469	1.00 20.00
ATOM	914	CB	GLU	A	921	38.047	56.940	23.011	1.00 20.00
ATOM	915	CG	GLU	A	921	38.258	57.743	21.736	1.00 20.00
ATOM	916	CD	GLU	A	921	39.404	58.696	21.848	1.00 20.00
ATOM	917	OE1	GLU	A	921	39.875	58.879	22.982	1.00 20.00
ATOM	918	OE2	GLU	A	921	39.836	59.261	20.825	1.00 20.00
ATOM	920	N	THR	A	922	37.936	53.893	21.615	1.00 20.00
ATOM	921	CA	THR	A	922	38.309	53.178	20.413	1.00 20.00
ATOM	922	C	THR	A	922	37.429	51.960	20.078	1.00 20.00
ATOM	923	O	THR	A	922	37.502	51.387	18.963	1.00 20.00
ATOM	924	CB	THR	A	922	39.742	52.728	20.559	1.00 20.00
ATOM	925	OG1	THR	A	922	40.441	53.058	19.366	1.00 20.00
ATOM	926	CG2	THR	A	922	39.824	51.214	20.816	1.00 20.00
ATOM	929	N	ASP	A	923	36.617	51.575	21.074	1.00 20.00
ATOM	930	CA	ASP	A	923	35.712	50.423	21.026	1.00 20.00
ATOM	931	C	ASP	A	923	34.972	50.387	22.350	1.00 20.00
ATOM	932	O	ASP	A	923	35.259	49.550	23.203	1.00 20.00
ATOM	933	CB	ASP	A	923	36.494	49.119	20.905	1.00 20.00
ATOM	934	CG	ASP	A	923	35.879	48.142	19.909	1.00 20.00
ATOM	935	OD1	ASP	A	923	35.624	48.553	18.745	1.00 20.00
ATOM	936	OD2	ASP	A	923	35.669	46.956	20.271	1.00 20.00
ATOM	938	N	PRO	A	924	34.042	51.323	22.577	1.00 20.00
ATOM	939	CA	PRO	A	924	33.362	51.211	23.874	1.00 20.00
ATOM	940	C	PRO	A	924	32.544	49.923	24.176	1.00 20.00
ATOM	941	O	PRO	A	924	32.172	49.720	25.342	1.00 20.00
ATOM	942	CB	PRO	A	924	32.540	52.506	23.953	1.00 20.00
ATOM	943	CG	PRO	A	924	33.214	53.417	22.960	1.00 20.00
ATOM	944	CD	PRO	A	924	33.600	52.512	21.841	1.00 20.00
ATOM	945	N	ALA	A	925	32.276	49.078	23.156	1.00 20.00
ATOM	946	CA	ALA	A	925	31.551	47.770	23.326	1.00 20.00
ATOM	947	C	ALA	A	925	32.438	46.878	24.193	1.00 20.00
ATOM	948	O	ALA	A	925	32.016	46.274	25.190	1.00 20.00
ATOM	949	CB	ALA	A	925	31.328	47.103	21.992	1.00 20.00
ATOM	951	N	PHE	A	926	33.695	46.843	23.771	1.00 20.00
ATOM	952	CA	PHE	A	926	34.782	46.173	24.431	1.00 20.00
ATOM	953	C	PHE	A	926	34.885	46.856	25.745	1.00 20.00
ATOM	954	O	PHE	A	926	34.896	46.269	26.772	1.00 20.00
ATOM	955	CB	PHE	A	926	36.058	46.460	23.667	1.00 20.00
ATOM	956	CG	PHE	A	926	37.046	45.347	23.693	1.00 20.00
ATOM	957	CD1	PHE	A	926	37.164	44.511	22.599	1.00 20.00
ATOM	958	CD2	PHE	A	926	37.810	45.127	24.825	1.00 20.00
ATOM	959	CE1	PHE	A	926	38.003	43.493	22.630	1.00 20.00
ATOM	960	CE2	PHE	A	926	38.661	44.107	24.881	1.00 20.00
ATOM	961	CZ	PHE	A	926	38.773	43.272	23.786	1.00 20.00
ATOM	963	N	ALA	A	927	35.024	48.154	25.681	1.00 20.00
ATOM	964	CA	ALA	A	927	35.084	48.926	26.885	1.00 20.00
ATOM	965	C	ALA	A	927	34.165	48.337	27.956	1.00 20.00
ATOM	966	O	ALA	A	927	34.695	47.721	28.843	1.00 20.00
ATOM	967	CB	ALA	A	927	34.717	50.348	26.587	1.00 20.00
ATOM	969	N	ILE	A	928	32.825	48.502	27.887	1.00 20.00
ATOM	970	CA	ILE	A	928	31.935	47.945	28.958	1.00 20.00
ATOM	971	C	ILE	A	928	31.760	46.437	29.001	1.00 20.00
ATOM	972	O	ILE	A	928	31.464	45.883	30.050	1.00 20.00
ATOM	973	CB	ILE	A	928	30.395	48.487	29.019	1.00 20.00
ATOM	974	CG1	ILE	A	928	30.081	49.486	27.941	1.00 20.00

FIG. 4N

```
ATOM    975  CG2 ILE A 928      30.098  49.114  30.414  1.00 20.00
ATOM    976  CD1 ILE A 928      29.952  50.862  28.545  1.00 20.00
ATOM    978  N   ALA A 929      31.895  45.782  27.860  1.00 20.00
ATOM    979  CA  ALA A 929      31.747  44.356  27.867  1.00 20.00
ATOM    980  C   ALA A 929      32.803  43.844  28.804  1.00 20.00
ATOM    981  O   ALA A 929      32.525  43.055  29.667  1.00 20.00
ATOM    982  CB  ALA A 929      31.946  43.823  26.510  1.00 20.00
ATOM    984  N   ASN A 930      34.010  44.358  28.642  1.00 20.00
ATOM    985  CA  ASN A 930      35.181  44.009  29.429  1.00 20.00
ATOM    986  C   ASN A 930      35.448  44.882  30.665  1.00 20.00
ATOM    987  O   ASN A 930      36.191  44.496  31.566  1.00 20.00
ATOM    988  CB  ASN A 930      36.397  44.067  28.511  1.00 20.00
ATOM    989  CG  ASN A 930      36.628  42.771  27.745  1.00 20.00
ATOM    990  OD1 ASN A 930      37.333  41.876  28.220  1.00 20.00
ATOM    991  ND2 ASN A 930      36.046  42.671  26.547  1.00 20.00
ATOM    995  N   SER A 931      34.847  46.063  30.695  1.00 20.00
ATOM    996  CA  SER A 931      35.050  47.041  31.768  1.00 20.00
ATOM    997  C   SER A 931      36.531  47.527  31.922  1.00 20.00
ATOM    998  O   SER A 931      37.074  47.556  33.020  1.00 20.00
ATOM    999  CB  SER A 931      34.541  46.453  33.084  1.00 20.00
ATOM   1000  OG  SER A 931      34.196  45.103  32.879  1.00 20.00
ATOM   1003  N   THR A 932      37.155  47.931  30.815  1.00 20.00
ATOM   1004  CA  THR A 932      38.545  48.392  30.821  1.00 20.00
ATOM   1005  C   THR A 932      38.800  49.536  29.872  1.00 20.00
ATOM   1006  O   THR A 932      38.184  49.614  28.803  1.00 20.00
ATOM   1007  CB  THR A 932      39.525  47.299  30.451  1.00 20.00
ATOM   1008  OG1 THR A 932      38.971  46.481  29.417  1.00 20.00
ATOM   1009  CG2 THR A 932      39.832  46.479  31.663  1.00 20.00
ATOM   1012  N   ALA A 933      39.747  50.384  30.287  1.00 20.00
ATOM   1013  CA  ALA A 933      40.179  51.608  29.597  1.00 20.00
ATOM   1014  C   ALA A 933      41.172  51.417  28.495  1.00 20.00
ATOM   1015  O   ALA A 933      41.155  52.134  27.513  1.00 20.00
ATOM   1016  CB  ALA A 933      40.778  52.547  30.597  1.00 20.00
ATOM   1018  N   SER A 934      42.086  50.480  28.709  1.00 20.00
ATOM   1019  CA  SER A 934      43.134  50.131  27.749  1.00 20.00
ATOM   1020  C   SER A 934      43.001  48.645  27.512  1.00 20.00
ATOM   1021  O   SER A 934      42.431  47.966  28.337  1.00 20.00
ATOM   1022  CB  SER A 934      44.511  50.396  28.374  1.00 20.00
ATOM   1023  OG  SER A 934      45.494  50.638  27.386  1.00 20.00
ATOM   1026  N   THR A 935      43.497  48.150  26.380  1.00 20.00
ATOM   1027  CA  THR A 935      43.529  46.701  26.144  1.00 20.00
ATOM   1028  C   THR A 935      44.801  46.297  26.814  1.00 20.00
ATOM   1029  O   THR A 935      45.015  45.118  27.082  1.00 20.00
ATOM   1030  CB  THR A 935      43.768  46.312  24.783  1.00 20.00
ATOM   1031  OG1 THR A 935      44.892  47.021  24.325  1.00 20.00
ATOM   1032  CG2 THR A 935      42.571  46.583  23.961  1.00 20.00
ATOM   1035  N   LEU A 936      45.640  47.301  27.070  1.00 20.00
ATOM   1036  CA  LEU A 936      46.897  47.138  27.735  1.00 20.00
ATOM   1037  C   LEU A 936      46.640  46.822  29.174  1.00 20.00
ATOM   1038  O   LEU A 936      45.579  47.010  29.666  1.00 20.00
ATOM   1039  CB  LEU A 936      47.699  48.413  27.635  1.00 20.00
ATOM   1040  CG  LEU A 936      47.921  49.086  26.273  1.00 20.00
ATOM   1041  CD1 LEU A 936      49.058  50.134  26.370  1.00 20.00
ATOM   1042  CD2 LEU A 936      48.250  48.029  25.238  1.00 20.00
ATOM   1044  N   SER A 937      47.652  46.322  29.841  1.00 20.00
ATOM   1045  CA  SER A 937      47.576  45.961  31.232  1.00 20.00
ATOM   1046  C   SER A 937      48.521  46.834  32.054  1.00 20.00
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FIG. 40

ATOM	1047	O	SER A 937	49.291	47.608	31.519	1.00	20.00
ATOM	1048	CB	SER A 937	47.988	44.501	31.384	1.00	20.00
ATOM	1049	OG	SER A 937	48.630	44.257	32.628	1.00	20.00
ATOM	1052	N	SER A 938	48.458	46.695	33.365	1.00	20.00
ATOM	1053	CA	SER A 938	49.319	47.433	34.239	1.00	20.00
ATOM	1054	C	SER A 938	50.724	46.904	33.957	1.00	20.00
ATOM	1055	O	SER A 938	51.686	47.668	33.847	1.00	20.00
ATOM	1056	CB	SER A 938	48.900	47.177	35.683	1.00	20.00
ATOM	1057	OG	SER A 938	50.012	47.071	36.555	1.00	20.00
ATOM	1060	N	GLN A 939	50.849	45.587	33.812	1.00	20.00
ATOM	1061	CA	GLN A 939	52.165	45.002	33.522	1.00	20.00
ATOM	1062	C	GLN A 939	52.709	45.435	32.165	1.00	20.00
ATOM	1063	O	GLN A 939	53.831	45.917	32.073	1.00	20.00
ATOM	1064	CB	GLN A 939	52.138	43.465	33.608	1.00	20.00
ATOM	1065	CG	GLN A 939	52.298	42.909	35.046	1.00	20.00
ATOM	1066	CD	GLN A 939	53.756	42.716	35.473	1.00	20.00
ATOM	1067	OE1	GLN A 939	54.595	42.185	34.711	1.00	20.00
ATOM	1068	NE2	GLN A 939	54.065	43.139	36.700	1.00	20.00
ATOM	1072	N	GLN A 940	51.932	45.294	31.111	1.00	20.00
ATOM	1073	CA	GLN A 940	52.445	45.696	29.813	1.00	20.00
ATOM	1074	C	GLN A 940	53.040	47.092	29.913	1.00	20.00
ATOM	1075	O	GLN A 940	53.944	47.477	29.163	1.00	20.00
ATOM	1076	CB	GLN A 940	51.330	45.696	28.788	1.00	20.00
ATOM	1077	CG	GLN A 940	51.695	46.374	27.506	1.00	20.00
ATOM	1078	CD	GLN A 940	52.703	45.592	26.720	1.00	20.00
ATOM	1079	OE1	GLN A 940	52.680	45.571	25.496	1.00	20.00
ATOM	1080	NE2	GLN A 940	53.591	44.934	27.418	1.00	20.00
ATOM	1084	N	LEU A 941	52.523	47.832	30.887	1.00	20.00
ATOM	1085	CA	LEU A 941	52.918	49.212	31.110	1.00	20.00
ATOM	1086	C	LEU A 941	54.285	49.397	31.744	1.00	20.00
ATOM	1087	O	LEU A 941	55.074	50.181	31.231	1.00	20.00
ATOM	1088	CB	LEU A 941	51.855	49.924	31.933	1.00	20.00
ATOM	1089	CG	LEU A 941	50.700	50.500	31.161	1.00	20.00
ATOM	1090	CD1	LEU A 941	50.187	51.653	31.924	1.00	20.00
ATOM	1091	CD2	LEU A 941	51.139	50.904	29.785	1.00	20.00
ATOM	1093	N	LEU A 942	54.571	48.720	32.848	1.00	20.00
ATOM	1094	CA	LEU A 942	55.882	48.863	33.431	1.00	20.00
ATOM	1095	C	LEU A 942	56.822	48.204	32.440	1.00	20.00
ATOM	1096	O	LEU A 942	57.987	48.583	32.283	1.00	20.00
ATOM	1097	CB	LEU A 942	55.955	48.147	34.756	1.00	20.00
ATOM	1098	CG	LEU A 942	54.731	48.399	35.609	1.00	20.00
ATOM	1099	CD1	LEU A 942	54.907	47.676	36.943	1.00	20.00
ATOM	1100	CD2	LEU A 942	54.526	49.936	35.793	1.00	20.00
ATOM	1102	N	HIS A 943	56.309	47.201	31.761	1.00	20.00
ATOM	1103	CA	HIS A 943	57.127	46.548	30.800	1.00	20.00
ATOM	1104	C	HIS A 943	57.754	47.596	29.894	1.00	20.00
ATOM	1105	O	HIS A 943	58.969	47.781	29.936	1.00	20.00
ATOM	1106	CB	HIS A 943	56.302	45.586	29.997	1.00	20.00
ATOM	1107	CG	HIS A 943	56.549	44.159	30.350	1.00	20.00
ATOM	1108	ND1	HIS A 943	56.709	43.732	31.649	1.00	20.00
ATOM	1109	CD2	HIS A 943	56.634	43.054	29.582	1.00	20.00
ATOM	1110	CE1	HIS A 943	56.881	42.427	31.670	1.00	20.00
ATOM	1111	NE2	HIS A 943	56.841	41.994	30.427	1.00	20.00
ATOM	1115	N	PHE A 944	56.929	48.278	29.084	1.00	20.00
ATOM	1116	CA	PHE A 944	57.396	49.327	28.162	1.00	20.00
ATOM	1117	C	PHE A 944	58.366	50.354	28.831	1.00	20.00
ATOM	1118	O	PHE A 944	59.368	50.775	28.249	1.00	20.00

FIG. 4P

ATOM	1119	CB	PHE	A	944	56.205	50.071	27.619	1.00 20.00
ATOM	1120	CG	PHE	A	944	55.484	49.372	26.515	1.00 20.00
ATOM	1121	CD1	PHE	A	944	54.116	49.207	26.572	1.00 20.00
ATOM	1122	CD2	PHE	A	944	56.130	49.020	25.368	1.00 20.00
ATOM	1123	CE1	PHE	A	944	53.432	48.727	25.515	1.00 20.00
ATOM	1124	CE2	PHE	A	944	55.433	48.534	24.300	1.00 20.00
ATOM	1125	CZ	PHE	A	944	54.096	48.393	24.375	1.00 20.00
ATOM	1127	N	ALA	A	945	58.055	50.749	30.057	1.00 20.00
ATOM	1128	CA	ALA	A	945	58.919	51.639	30.792	1.00 20.00
ATOM	1129	C	ALA	A	945	60.323	51.010	31.013	1.00 20.00
ATOM	1130	O	ALA	A	945	61.349	51.690	30.906	1.00 20.00
ATOM	1131	CB	ALA	A	945	58.292	51.974	32.101	1.00 20.00
ATOM	1133	N	ALA	A	946	60.373	49.710	31.297	1.00 20.00
ATOM	1134	CA	ALA	A	946	61.650	49.043	31.547	1.00 20.00
ATOM	1135	C	ALA	A	946	62.466	48.605	30.330	1.00 20.00
ATOM	1136	O	ALA	A	946	63.646	48.331	30.434	1.00 20.00
ATOM	1137	CB	ALA	A	946	61.418	47.872	32.429	1.00 20.00
ATOM	1139	N	ASP	A	947	61.823	48.486	29.188	1.00 20.00
ATOM	1140	CA	ASP	A	947	62.532	48.106	27.998	1.00 20.00
ATOM	1141	C	ASP	A	947	63.351	49.335	27.765	1.00 20.00
ATOM	1142	O	ASP	A	947	64.564	49.273	27.560	1.00 20.00
ATOM	1143	CB	ASP	A	947	61.560	47.930	26.849	1.00 20.00
ATOM	1144	CG	ASP	A	947	61.242	46.473	26.549	1.00 20.00
ATOM	1145	OD1	ASP	A	947	61.770	45.561	27.247	1.00 20.00
ATOM	1146	OD2	ASP	A	947	60.447	46.255	25.595	1.00 20.00
ATOM	1148	N	VAL	A	948	62.640	50.465	27.811	1.00 20.00
ATOM	1149	CA	VAL	A	948	63.203	51.808	27.624	1.00 20.00
ATOM	1150	C	VAL	A	948	64.337	52.099	28.598	1.00 20.00
ATOM	1151	O	VAL	A	948	65.360	52.539	28.177	1.00 20.00
ATOM	1152	CB	VAL	A	948	62.108	52.917	27.776	1.00 20.00
ATOM	1153	CG1	VAL	A	948	62.712	54.286	27.666	1.00 20.00
ATOM	1154	CG2	VAL	A	948	61.121	52.784	26.722	1.00 20.00
ATOM	1156	N	ALA	A	949	64.166	51.850	29.886	1.00 20.00
ATOM	1157	CA	ALA	A	949	65.243	52.135	30.812	1.00 20.00
ATOM	1158	C	ALA	A	949	66.449	51.321	30.460	1.00 20.00
ATOM	1159	O	ALA	A	949	67.578	51.738	30.669	1.00 20.00
ATOM	1160	CB	ALA	A	949	64.850	51.822	32.209	1.00 20.00
ATOM	1162	N	ARG	A	950	66.212	50.134	29.928	1.00 20.00
ATOM	1163	CA	ARG	A	950	67.293	49.254	29.578	1.00 20.00
ATOM	1164	C	ARG	A	950	68.005	49.853	28.406	1.00 20.00
ATOM	1165	O	ARG	A	950	69.110	50.330	28.534	1.00 20.00
ATOM	1166	CB	ARG	A	950	66.762	47.872	29.240	1.00 20.00
ATOM	1167	CG	ARG	A	950	67.029	46.827	30.351	1.00 20.00
ATOM	1168	CD	ARG	A	950	67.033	45.384	29.809	1.00 20.00
ATOM	1169	NE	ARG	A	950	65.891	45.157	28.900	1.00 20.00
ATOM	1170	CZ	ARG	A	950	64.646	44.807	29.260	1.00 20.00
ATOM	1171	NH1	ARG	A	950	64.301	44.610	30.522	1.00 20.00
ATOM	1172	NH2	ARG	A	950	63.726	44.693	28.323	1.00 20.00
ATOM	1179	N	GLY	A	951	67.390	49.844	27.248	1.00 20.00
ATOM	1180	CA	GLY	A	951	68.105	50.427	26.146	1.00 20.00
ATOM	1181	C	GLY	A	951	68.769	51.722	26.564	1.00 20.00
ATOM	1182	O	GLY	A	951	69.885	52.024	26.163	1.00 20.00
ATOM	1184	N	MET	A	952	68.080	52.500	27.386	1.00 20.00
ATOM	1185	CA	MET	A	952	68.605	53.787	27.807	1.00 20.00
ATOM	1186	C	MET	A	952	69.952	53.633	28.437	1.00 20.00
ATOM	1187	O	MET	A	952	70.949	53.969	27.845	1.00 20.00
ATOM	1188	CB	MET	A	952	67.659	54.492	28.797	1.00 20.00

FIG. 4Q

ATOM	1189	CG	MET	A	952	67.289	55.894	28.400	1.00	20.00
ATOM	1190	SD	MET	A	952	67.360	56.078	26.632	1.00	20.00
ATOM	1191	CE	MET	A	952	68.656	57.374	26.554	1.00	20.00
ATOM	1193	N	ASP	A	953	69.903	53.096	29.648	1.00	20.00
ATOM	1194	CA	ASP	A	953	70.999	52.819	30.539	1.00	20.00
ATOM	1195	C	ASP	A	953	72.126	52.077	29.948	1.00	20.00
ATOM	1196	O	ASP	A	953	73.077	51.814	30.608	1.00	20.00
ATOM	1197	CB	ASP	A	953	70.496	52.036	31.733	1.00	20.00
ATOM	1198	CG	ASP	A	953	71.538	51.117	32.295	1.00	20.00
ATOM	1199	OD1	ASP	A	953	72.241	51.480	33.245	1.00	20.00
ATOM	1200	OD2	ASP	A	953	71.672	50.004	31.785	1.00	20.00
ATOM	1202	N	TYR	A	954	72.025	51.743	28.692	1.00	20.00
ATOM	1203	CA	TYR	A	954	73.060	51.020	28.034	1.00	20.00
ATOM	1204	C	TYR	A	954	73.930	52.011	27.324	1.00	20.00
ATOM	1205	O	TYR	A	954	75.135	51.833	27.254	1.00	20.00
ATOM	1206	CB	TYR	A	954	72.416	50.047	27.070	1.00	20.00
ATOM	1207	CG	TYR	A	954	73.330	49.432	26.068	1.00	20.00
ATOM	1208	CD1	TYR	A	954	74.294	48.485	26.442	1.00	20.00
ATOM	1209	CD2	TYR	A	954	73.181	49.719	24.734	1.00	20.00
ATOM	1210	CE1	TYR	A	954	75.071	47.839	25.483	1.00	20.00
ATOM	1211	CE2	TYR	A	954	73.947	49.082	23.779	1.00	20.00
ATOM	1212	CZ	TYR	A	954	74.883	48.136	24.153	1.00	20.00
ATOM	1213	OH	TYR	A	954	75.525	47.442	23.152	1.00	20.00
ATOM	1216	N	LEU	A	955	73.286	53.052	26.786	1.00	20.00
ATOM	1217	CA	LEU	A	955	73.908	54.184	26.069	1.00	20.00
ATOM	1218	C	LEU	A	955	74.356	55.110	27.176	1.00	20.00
ATOM	1219	O	LEU	A	955	75.441	55.609	27.207	1.00	20.00
ATOM	1220	CB	LEU	A	955	72.863	54.943	25.265	1.00	20.00
ATOM	1221	CG	LEU	A	955	72.005	54.277	24.181	1.00	20.00
ATOM	1222	CD1	LEU	A	955	70.489	54.637	24.288	1.00	20.00
ATOM	1223	CD2	LEU	A	955	72.573	54.751	22.838	1.00	20.00
ATOM	1225	N	SER	A	956	73.465	55.311	28.113	1.00	20.00
ATOM	1226	CA	SER	A	956	73.699	56.176	29.209	1.00	20.00
ATOM	1227	C	SER	A	956	74.985	55.783	29.829	1.00	20.00
ATOM	1228	O	SER	A	956	75.557	56.555	30.600	1.00	20.00
ATOM	1229	CB	SER	A	956	72.534	56.068	30.172	1.00	20.00
ATOM	1230	OG	SER	A	956	72.960	56.102	31.513	1.00	20.00
ATOM	1233	N	GLN	A	957	75.468	54.594	29.495	1.00	20.00
ATOM	1234	CA	GLN	A	957	76.755	54.097	30.040	1.00	20.00
ATOM	1235	C	GLN	A	957	77.824	54.054	28.959	1.00	20.00
ATOM	1236	O	GLN	A	957	78.985	54.213	29.208	1.00	20.00
ATOM	1237	CB	GLN	A	957	76.591	52.703	30.617	1.00	20.00
ATOM	1238	CG	GLN	A	957	75.563	52.626	31.692	1.00	20.00
ATOM	1239	CD	GLN	A	957	76.088	51.882	32.875	1.00	20.00
ATOM	1240	OE1	GLN	A	957	77.083	52.314	33.492	1.00	20.00
ATOM	1241	NE2	GLN	A	957	75.447	50.747	33.215	1.00	20.00
ATOM	1245	N	LYS	A	958	77.396	53.827	27.747	1.00	20.00
ATOM	1246	CA	LYS	A	958	78.273	53.813	26.622	1.00	20.00
ATOM	1247	C	LYS	A	958	78.801	55.275	26.542	1.00	20.00
ATOM	1248	O	LYS	A	958	79.643	55.627	25.704	1.00	20.00
ATOM	1249	CB	LYS	A	958	77.427	53.440	25.379	1.00	20.00
ATOM	1250	CG	LYS	A	958	78.110	52.552	24.355	1.00	20.00
ATOM	1251	CD	LYS	A	958	78.715	51.303	25.011	1.00	20.00
ATOM	1252	CE	LYS	A	958	77.845	50.099	24.743	1.00	20.00
ATOM	1253	NZ	LYS	A	958	77.570	50.041	23.271	1.00	20.00
ATOM	1258	N	GLN	A	959	78.268	56.108	27.438	1.00	20.00
ATOM	1259	CA	GLN	A	959	78.526	57.551	27.543	1.00	20.00

FIG. 4R

```
ATOM   1260  C   GLN A 959      77.366  58.361  26.838  1.00 20.00
ATOM   1261  O   GLN A 959      76.848  59.327  27.401  1.00 20.00
ATOM   1262  CB  GLN A 959      79.901  57.893  26.973  1.00 20.00
ATOM   1263  CG  GLN A 959      80.490  59.183  27.492  1.00 20.00
ATOM   1264  CD  GLN A 959      80.934  59.114  28.944  1.00 20.00
ATOM   1265  OE1 GLN A 959      81.840  58.313  29.295  1.00 20.00
ATOM   1266  NE2 GLN A 959      80.332  59.979  29.811  1.00 20.00
ATOM   1270  N   PHE A 960      76.937  57.940  25.649  1.00 20.00
ATOM   1271  CA  PHE A 960      75.828  58.582  24.898  1.00 20.00
ATOM   1272  C   PHE A 960      74.667  59.365  25.618  1.00 20.00
ATOM   1273  O   PHE A 960      74.110  58.916  26.628  1.00 20.00
ATOM   1274  CB  PHE A 960      75.189  57.528  23.985  1.00 20.00
ATOM   1275  CG  PHE A 960      76.070  57.067  22.851  1.00 20.00
ATOM   1276  CD1 PHE A 960      76.570  55.766  22.818  1.00 20.00
ATOM   1277  CD2 PHE A 960      76.367  57.901  21.792  1.00 20.00
ATOM   1278  CE1 PHE A 960      77.349  55.308  21.743  1.00 20.00
ATOM   1279  CE2 PHE A 960      77.148  57.442  20.720  1.00 20.00
ATOM   1280  CZ  PHE A 960      77.636  56.142  20.704  1.00 20.00
ATOM   1282  N   ILE A 961      74.308  60.532  25.068  1.00 20.00
ATOM   1283  CA  ILE A 961      73.212  61.377  25.623  1.00 20.00
ATOM   1284  C   ILE A 961      72.076  61.460  24.611  1.00 20.00
ATOM   1285  O   ILE A 961      72.341  61.698  23.434  1.00 20.00
ATOM   1286  CB  ILE A 961      73.631  62.832  25.918  1.00 20.00
ATOM   1287  CG1 ILE A 961      74.862  62.886  26.840  1.00 20.00
ATOM   1288  CG2 ILE A 961      72.489  63.547  26.600  1.00 20.00
ATOM   1289  CD1 ILE A 961      75.935  63.855  26.373  1.00 20.00
ATOM   1291  N   HIS A 962      70.821  61.314  25.049  1.00 20.00
ATOM   1292  CA  HIS A 962      69.704  61.307  24.088  1.00 20.00
ATOM   1293  C   HIS A 962      69.158  62.604  23.535  1.00 20.00
ATOM   1294  O   HIS A 962      69.296  62.872  22.344  1.00 20.00
ATOM   1295  CB  HIS A 962      68.515  60.516  24.641  1.00 20.00
ATOM   1296  CG  HIS A 962      67.658  59.896  23.580  1.00 20.00
ATOM   1297  ND1 HIS A 962      67.259  58.586  23.621  1.00 20.00
ATOM   1298  CD2 HIS A 962      67.192  60.388  22.416  1.00 20.00
ATOM   1299  CE1 HIS A 962      66.589  58.290  22.528  1.00 20.00
ATOM   1300  NE2 HIS A 962      66.538  59.369  21.780  1.00 20.00
ATOM   1304  N   ARG A 963      68.502  63.363  24.413  1.00 20.00
ATOM   1305  CA  ARG A 963      67.848  64.665  24.122  1.00 20.00
ATOM   1306  C   ARG A 963      66.653  64.636  23.125  1.00 20.00
ATOM   1307  O   ARG A 963      66.561  65.380  22.147  1.00 20.00
ATOM   1308  CB  ARG A 963      68.909  65.724  23.726  1.00 20.00
ATOM   1309  CG  ARG A 963      69.366  65.645  22.334  1.00 20.00
ATOM   1310  CD  ARG A 963      70.710  66.180  22.216  1.00 20.00
ATOM   1311  NE  ARG A 963      71.391  65.521  21.127  1.00 20.00
ATOM   1312  CZ  ARG A 963      71.002  65.603  19.873  1.00 20.00
ATOM   1313  NH1 ARG A 963      69.946  66.323  19.584  1.00 20.00
ATOM   1314  NH2 ARG A 963      71.648  64.941  18.925  1.00 20.00
ATOM   1321  N   ASN A 964      65.705  63.767  23.408  1.00 20.00
ATOM   1322  CA  ASN A 964      64.536  63.623  22.545  1.00 20.00
ATOM   1323  C   ASN A 964      63.904  62.262  22.803  1.00 20.00
ATOM   1324  O   ASN A 964      63.497  61.558  21.890  1.00 20.00
ATOM   1325  CB  ASN A 964      64.890  63.763  21.054  1.00 20.00
ATOM   1326  CG  ASN A 964      63.647  63.940  20.206  1.00 20.00
ATOM   1327  OD1 ASN A 964      62.565  64.079  20.780  1.00 20.00
ATOM   1328  ND2 ASN A 964      63.769  63.939  18.866  1.00 20.00
ATOM   1332  N   LEU A 965      63.861  61.914  24.081  1.00 20.00
ATOM   1333  CA  LEU A 965      63.291  60.665  24.546  1.00 20.00
```

FIG. 4S

ATOM	1334	C	LEU	A	965	61.884	61.116	24.926	1.00 20.00
ATOM	1335	O	LEU	A	965	61.701	62.119	25.629	1.00 20.00
ATOM	1336	CB	LEU	A	965	64.079	60.172	25.769	1.00 20.00
ATOM	1337	CG	LEU	A	965	64.292	58.716	26.189	1.00 20.00
ATOM	1338	CD1	LEU	A	965	64.689	57.802	25.040	1.00 20.00
ATOM	1339	CD2	LEU	A	965	65.320	58.728	27.276	1.00 20.00
ATOM	1341	N	ALA	A	966	60.905	60.381	24.412	1.00 20.00
ATOM	1342	CA	ALA	A	966	59.511	60.666	24.605	1.00 20.00
ATOM	1343	C	ALA	A	966	58.812	59.674	23.677	1.00 20.00
ATOM	1344	O	ALA	A	966	59.379	59.250	22.667	1.00 20.00
ATOM	1345	CB	ALA	A	966	59.244	62.056	24.189	1.00 20.00
ATOM	1347	N	ALA	A	967	57.581	59.320	24.014	1.00 20.00
ATOM	1348	CA	ALA	A	967	56.826	58.358	23.242	1.00 20.00
ATOM	1349	C	ALA	A	967	56.842	58.489	21.740	1.00 20.00
ATOM	1350	O	ALA	A	967	57.050	57.521	21.044	1.00 20.00
ATOM	1351	CB	ALA	A	967	55.375	58.306	23.721	1.00 20.00
ATOM	1353	N	ARG	A	968	56.606	59.671	21.205	1.00 20.00
ATOM	1354	CA	ARG	A	968	56.580	59.697	19.759	1.00 20.00
ATOM	1355	C	ARG	A	968	57.802	59.015	19.160	1.00 20.00
ATOM	1356	O	ARG	A	968	57.751	58.532	18.041	1.00 20.00
ATOM	1357	CB	ARG	A	968	56.455	61.123	19.226	1.00 20.00
ATOM	1358	CG	ARG	A	968	57.264	62.162	19.987	1.00 20.00
ATOM	1359	CD	ARG	A	968	57.684	63.354	19.087	1.00 20.00
ATOM	1360	NE	ARG	A	968	58.467	64.376	19.784	1.00 20.00
ATOM	1361	CZ	ARG	A	968	58.098	64.982	20.904	1.00 20.00
ATOM	1362	NH1	ARG	A	968	56.937	64.698	21.492	1.00 20.00
ATOM	1363	NH2	ARG	A	968	58.929	65.828	21.473	1.00 20.00
ATOM	1370	N	ASN	A	969	58.881	58.913	19.931	1.00 20.00
ATOM	1371	CA	ASN	A	969	60.122	58.388	19.383	1.00 20.00
ATOM	1372	C	ASN	A	969	60.608	57.008	19.754	1.00 20.00
ATOM	1373	O	ASN	A	969	61.716	56.647	19.413	1.00 20.00
ATOM	1374	CB	ASN	A	969	61.232	59.407	19.630	1.00 20.00
ATOM	1375	CG	ASN	A	969	60.873	60.787	19.118	1.00 20.00
ATOM	1376	OD1	ASN	A	969	60.733	61.724	19.892	1.00 20.00
ATOM	1377	ND2	ASN	A	969	60.702	60.910	17.802	1.00 20.00
ATOM	1381	N	ILE	A	970	59.775	56.249	20.443	1.00 20.00
ATOM	1382	CA	ILE	A	970	60.073	54.912	20.851	1.00 20.00
ATOM	1383	C	ILE	A	970	59.153	54.057	20.034	1.00 20.00
ATOM	1384	O	ILE	A	970	58.006	54.384	19.930	1.00 20.00
ATOM	1385	CB	ILE	A	970	59.717	54.770	22.294	1.00 20.00
ATOM	1386	CG1	ILE	A	970	60.699	55.565	23.110	1.00 20.00
ATOM	1387	CG2	ILE	A	970	59.730	53.328	22.724	1.00 20.00
ATOM	1388	CD1	ILE	A	970	60.800	55.095	24.515	1.00 20.00
ATOM	1390	N	LEU	A	971	59.626	52.971	19.435	1.00 20.00
ATOM	1391	CA	LEU	A	971	58.733	52.086	18.656	1.00 20.00
ATOM	1392	C	LEU	A	971	58.290	50.891	19.444	1.00 20.00
ATOM	1393	O	LEU	A	971	58.776	50.653	20.523	1.00 20.00
ATOM	1394	CB	LEU	A	971	59.422	51.582	17.418	1.00 20.00
ATOM	1395	CG	LEU	A	971	59.930	52.837	16.785	1.00 20.00
ATOM	1396	CD1	LEU	A	971	61.161	52.652	16.019	1.00 20.00
ATOM	1397	CD2	LEU	A	971	58.844	53.290	15.909	1.00 20.00
ATOM	1399	N	VAL	A	972	57.305	50.171	18.929	1.00 20.00
ATOM	1400	CA	VAL	A	972	56.894	48.941	19.594	1.00 20.00
ATOM	1401	C	VAL	A	972	57.044	47.883	18.541	1.00 20.00
ATOM	1402	O	VAL	A	972	56.221	47.793	17.661	1.00 20.00
ATOM	1403	CB	VAL	A	972	55.492	48.932	20.043	1.00 20.00
ATOM	1404	CG1	VAL	A	972	55.224	47.588	20.632	1.00 20.00

FIG. 4T

ATOM	1405	CG2	VAL	A	972	55.264	50.012	21.107	1.00	20.00
ATOM	1407	N	GLY	A	973	58.127	47.106	18.614	1.00	20.00
ATOM	1408	CA	GLY	A	973	58.375	46.109	17.614	1.00	20.00
ATOM	1409	C	GLY	A	973	58.065	44.685	17.980	1.00	20.00
ATOM	1410	O	GLY	A	973	57.370	44.393	18.927	1.00	20.00
ATOM	1412	N	GLU	A	974	58.612	43.793	17.178	1.00	20.00
ATOM	1413	CA	GLU	A	974	58.445	42.383	17.357	1.00	20.00
ATOM	1414	C	GLU	A	974	58.379	41.981	18.795	1.00	20.00
ATOM	1415	O	GLU	A	974	59.246	42.274	19.572	1.00	20.00
ATOM	1416	CB	GLU	A	974	59.568	41.648	16.671	1.00	20.00
ATOM	1417	CG	GLU	A	974	59.187	41.010	15.343	1.00	20.00
ATOM	1418	CD	GLU	A	974	57.698	41.173	14.936	1.00	20.00
ATOM	1419	OE1	GLU	A	974	56.763	40.870	15.733	1.00	20.00
ATOM	1420	OE2	GLU	A	974	57.467	41.592	13.780	1.00	20.00
ATOM	1422	N	ASN	A	975	57.305	41.316	19.147	1.00	20.00
ATOM	1423	CA	ASN	A	975	57.119	40.830	20.483	1.00	20.00
ATOM	1424	C	ASN	A	975	56.741	41.832	21.554	1.00	20.00
ATOM	1425	O	ASN	A	975	56.811	41.544	22.758	1.00	20.00
ATOM	1426	CB	ASN	A	975	58.333	40.006	20.864	1.00	20.00
ATOM	1427	CG	ASN	A	975	58.189	38.519	20.428	1.00	20.00
ATOM	1428	OD1	ASN	A	975	58.243	37.639	21.263	1.00	20.00
ATOM	1429	ND2	ASN	A	975	57.988	38.266	19.136	1.00	20.00
ATOM	1433	N	TYR	A	976	56.299	43.003	21.103	1.00	20.00
ATOM	1434	CA	TYR	A	976	55.839	44.047	21.988	1.00	20.00
ATOM	1435	C	TYR	A	976	56.946	44.589	22.839	1.00	20.00
ATOM	1436	O	TYR	A	976	56.797	44.863	24.016	1.00	20.00
ATOM	1437	CB	TYR	A	976	54.684	43.498	22.830	1.00	20.00
ATOM	1438	CG	TYR	A	976	53.466	43.191	21.993	1.00	20.00
ATOM	1439	CD1	TYR	A	976	52.878	41.927	22.017	1.00	20.00
ATOM	1440	CD2	TYR	A	976	52.939	44.157	21.112	1.00	20.00
ATOM	1441	CE1	TYR	A	976	51.801	41.624	21.182	1.00	20.00
ATOM	1442	CE2	TYR	A	976	51.874	43.870	20.279	1.00	20.00
ATOM	1443	CZ	TYR	A	976	51.306	42.604	20.307	1.00	20.00
ATOM	1444	OH	TYR	A	976	50.273	42.291	19.427	1.00	20.00
ATOM	1447	N	VAL	A	977	58.070	44.787	22.191	1.00	20.00
ATOM	1448	CA	VAL	A	977	59.260	45.295	22.845	1.00	20.00
ATOM	1449	C	VAL	A	977	59.536	46.766	22.497	1.00	20.00
ATOM	1450	O	VAL	A	977	59.446	47.195	21.355	1.00	20.00
ATOM	1451	CB	VAL	A	977	60.514	44.377	22.485	1.00	20.00
ATOM	1452	CG1	VAL	A	977	61.768	44.854	23.182	1.00	20.00
ATOM	1453	CG2	VAL	A	977	60.230	42.943	22.890	1.00	20.00
ATOM	1455	N	ALA	A	978	59.839	47.529	23.525	1.00	20.00
ATOM	1456	CA	ALA	A	978	60.174	48.898	23.328	1.00	20.00
ATOM	1457	C	ALA	A	978	61.434	48.921	22.476	1.00	20.00
ATOM	1458	O	ALA	A	978	62.242	48.026	22.527	1.00	20.00
ATOM	1459	CB	ALA	A	978	60.423	49.546	24.643	1.00	20.00
ATOM	1461	N	LYS	A	979	61.597	49.926	21.653	1.00	20.00
ATOM	1462	CA	LYS	A	979	62.791	50.005	20.864	1.00	20.00
ATOM	1463	C	LYS	A	979	63.098	51.476	20.826	1.00	20.00
ATOM	1464	O	LYS	A	979	62.263	52.262	20.387	1.00	20.00
ATOM	1465	CB	LYS	A	979	62.551	49.492	19.448	1.00	20.00
ATOM	1466	CG	LYS	A	979	62.076	48.043	19.369	1.00	20.00
ATOM	1467	CD	LYS	A	979	63.115	47.009	19.864	1.00	20.00
ATOM	1468	CE	LYS	A	979	63.866	46.343	18.708	1.00	20.00
ATOM	1469	NZ	LYS	A	979	63.212	45.122	18.253	1.00	20.00
ATOM	1474	N	ILE	A	980	64.274	51.873	21.302	1.00	20.00
ATOM	1475	CA	ILE	A	980	64.615	53.287	21.240	1.00	20.00

FIG. 4U

ATOM	1476	C	ILE	A	980	65.131	53.691	19.858	1.00	20.00
ATOM	1477	O	ILE	A	980	65.938	53.004	19.233	1.00	20.00
ATOM	1478	CB	ILE	A	980	65.671	53.665	22.263	1.00	20.00
ATOM	1479	CG1	ILE	A	980	65.205	53.311	23.667	1.00	20.00
ATOM	1480	CG2	ILE	A	980	65.943	55.135	22.173	1.00	20.00
ATOM	1481	CD1	ILE	A	980	66.262	53.521	24.730	1.00	20.00
ATOM	1483	N	ALA	A	981	64.629	54.815	19.383	1.00	20.00
ATOM	1484	CA	ALA	A	981	65.038	55.342	18.097	1.00	20.00
ATOM	1485	C	ALA	A	981	65.244	56.854	18.141	1.00	20.00
ATOM	1486	O	ALA	A	981	65.039	57.530	19.172	1.00	20.00
ATOM	1487	CB	ALA	A	981	64.024	55.024	17.060	1.00	20.00
ATOM	1489	N	ASP	A	982	65.610	57.362	16.973	1.00	20.00
ATOM	1490	CA	ASP	A	982	65.888	58.763	16.721	1.00	20.00
ATOM	1491	C	ASP	A	982	66.653	59.517	17.801	1.00	20.00
ATOM	1492	O	ASP	A	982	66.041	60.135	18.684	1.00	20.00
ATOM	1493	CB	ASP	A	982	64.620	59.527	16.416	1.00	20.00
ATOM	1494	CG	ASP	A	982	64.911	60.946	16.122	1.00	20.00
ATOM	1495	OD1	ASP	A	982	65.455	61.240	15.031	1.00	20.00
ATOM	1496	OD2	ASP	A	982	64.626	61.766	16.998	1.00	20.00
ATOM	1498	N	PHE	A	983	67.988	59.525	17.706	1.00	20.00
ATOM	1499	CA	PHE	A	983	68.770	60.223	18.733	1.00	20.00
ATOM	1500	C	PHE	A	983	70.123	60.755	18.312	1.00	20.00
ATOM	1501	O	PHE	A	983	70.565	60.712	17.155	1.00	20.00
ATOM	1502	CB	PHE	A	983	69.001	59.327	19.948	1.00	20.00
ATOM	1503	CG	PHE	A	983	69.411	57.928	19.589	1.00	20.00
ATOM	1504	CD1	PHE	A	983	68.856	57.280	18.452	1.00	20.00
ATOM	1505	CD2	PHE	A	983	70.310	57.244	20.375	1.00	20.00
ATOM	1506	CE1	PHE	A	983	69.181	55.987	18.106	1.00	20.00
ATOM	1507	CE2	PHE	A	983	70.648	55.939	20.044	1.00	20.00
ATOM	1508	CZ	PHE	A	983	70.075	55.308	18.895	1.00	20.00
ATOM	1510	N	GLY	A	984	70.797	61.274	19.305	1.00	20.00
ATOM	1511	CA	GLY	A	984	72.082	61.799	19.010	1.00	20.00
ATOM	1512	C	GLY	A	984	73.058	60.661	18.913	1.00	20.00
ATOM	1513	O	GLY	A	984	72.980	59.633	19.633	1.00	20.00
ATOM	1515	N	LEU	A	985	73.978	60.846	17.977	1.00	20.00
ATOM	1516	CA	LEU	A	985	75.055	59.913	17.812	1.00	20.00
ATOM	1517	C	LEU	A	985	76.044	60.741	18.669	1.00	20.00
ATOM	1518	O	LEU	A	985	77.236	60.872	18.323	1.00	20.00
ATOM	1519	CB	LEU	A	985	75.483	59.871	16.342	1.00	20.00
ATOM	1520	CG	LEU	A	985	75.093	58.770	15.337	1.00	20.00
ATOM	1521	CD1	LEU	A	985	75.645	57.463	15.830	1.00	20.00
ATOM	1522	CD2	LEU	A	985	73.579	58.659	15.129	1.00	20.00
ATOM	1524	N	SER	A	986	75.561	61.306	19.786	1.00	20.00
ATOM	1525	CA	SER	A	986	76.443	62.118	20.611	1.00	20.00
ATOM	1526	C	SER	A	986	76.926	61.629	21.970	1.00	20.00
ATOM	1527	O	SER	A	986	76.169	61.709	22.937	1.00	20.00
ATOM	1528	CB	SER	A	986	75.850	63.504	20.815	1.00	20.00
ATOM	1529	OG	SER	A	986	76.764	64.504	20.379	1.00	20.00
ATOM	1532	N	ARG	A	987	78.189	61.152	22.037	1.00	20.00
ATOM	1533	CA	ARG	A	987	78.763	60.709	23.306	1.00	20.00
ATOM	1534	C	ARG	A	987	79.511	61.893	23.794	1.00	20.00
ATOM	1535	O	ARG	A	987	80.191	62.578	23.059	1.00	20.00
ATOM	1536	CB	ARG	A	987	79.752	59.525	23.214	1.00	20.00
ATOM	1537	CG	ARG	A	987	79.583	58.534	22.078	1.00	20.00
ATOM	1538	CD	ARG	A	987	80.953	58.120	21.459	1.00	20.00
ATOM	1539	NE	ARG	A	987	81.908	57.509	22.396	1.00	20.00
ATOM	1540	CZ	ARG	A	987	82.932	56.731	22.021	1.00	20.00

FIG. 4V

ATOM	1541	NH1	ARG	A	987	83.127	56.473	20.738	1.00	20.00
ATOM	1542	NH2	ARG	A	987	83.761	56.206	22.936	1.00	20.00
ATOM	1549	N	GLY	A	988	79.387	62.122	25.068	1.00	20.00
ATOM	1550	CA	GLY	A	988	80.028	63.260	25.633	1.00	20.00
ATOM	1551	C	GLY	A	988	79.480	63.223	27.024	1.00	20.00
ATOM	1552	O	GLY	A	988	79.050	62.151	27.453	1.00	20.00
ATOM	1554	N	GLN	A	989	79.521	64.369	27.704	1.00	20.00
ATOM	1555	CA	GLN	A	989	79.020	64.579	29.053	1.00	20.00
ATOM	1556	C	GLN	A	989	78.115	65.864	29.062	1.00	20.00
ATOM	1557	O	GLN	A	989	77.565	66.257	30.075	1.00	20.00
ATOM	1558	CB	GLN	A	989	80.219	64.739	29.974	1.00	20.00
ATOM	1559	CG	GLN	A	989	79.924	65.292	31.348	1.00	20.00
ATOM	1560	CD	GLN	A	989	81.068	66.095	31.985	1.00	20.00
ATOM	1561	OE1	GLN	A	989	81.783	66.897	31.332	1.00	20.00
ATOM	1562	NE2	GLN	A	989	81.233	65.891	33.273	1.00	20.00
ATOM	1566	N	GLU	A	990	77.933	66.496	27.908	1.00	20.00
ATOM	1567	CA	GLU	A	990	77.185	67.704	27.889	1.00	20.00
ATOM	1568	C	GLU	A	990	76.348	68.030	26.675	1.00	20.00
ATOM	1569	O	GLU	A	990	75.199	68.420	26.836	1.00	20.00
ATOM	1570	CB	GLU	A	990	78.134	68.853	28.117	1.00	20.00
ATOM	1571	CG	GLU	A	990	78.194	69.367	29.499	1.00	20.00
ATOM	1572	CD	GLU	A	990	79.467	68.991	30.151	1.00	20.00
ATOM	1573	OE1	GLU	A	990	80.437	68.623	29.443	1.00	20.00
ATOM	1574	OE2	GLU	A	990	79.486	69.061	31.387	1.00	20.00
ATOM	1576	N	VAL	A	991	76.878	67.895	25.469	1.00	20.00
ATOM	1577	CA	VAL	A	991	76.098	68.270	24.274	1.00	20.00
ATOM	1578	C	VAL	A	991	75.373	69.616	24.400	1.00	20.00
ATOM	1579	O	VAL	A	991	74.538	69.823	25.274	1.00	20.00
ATOM	1580	CB	VAL	A	991	74.965	67.324	23.910	1.00	20.00
ATOM	1581	CG1	VAL	A	991	74.620	67.527	22.479	1.00	20.00
ATOM	1582	CG2	VAL	A	991	75.323	65.922	24.159	1.00	20.00
ATOM	1584	N	TYR	A	992	75.674	70.528	23.504	1.00	20.00
ATOM	1585	CA	TYR	A	992	74.997	71.780	23.514	1.00	20.00
ATOM	1586	C	TYR	A	992	74.389	71.784	22.118	1.00	20.00
ATOM	1587	O	TYR	A	992	75.036	71.437	21.138	1.00	20.00
ATOM	1588	CB	TYR	A	992	76.003	72.945	23.687	1.00	20.00
ATOM	1589	CG	TYR	A	992	75.520	74.227	23.027	1.00	20.00
ATOM	1590	CD1	TYR	A	992	74.579	75.023	23.654	1.00	20.00
ATOM	1591	CD2	TYR	A	992	75.804	74.487	21.702	1.00	20.00
ATOM	1592	CE1	TYR	A	992	73.939	75.989	22.987	1.00	20.00
ATOM	1593	CE2	TYR	A	992	75.160	75.453	21.044	1.00	20.00
ATOM	1594	CZ	TYR	A	992	74.218	76.200	21.690	1.00	20.00
ATOM	1595	OH	TYR	A	992	73.552	77.196	21.023	1.00	20.00
ATOM	1598	N	VAL	A	993	73.131	72.161	22.020	1.00	20.00
ATOM	1599	CA	VAL	A	993	72.482	72.226	20.712	1.00	20.00
ATOM	1600	C	VAL	A	993	71.311	73.168	21.008	1.00	20.00
ATOM	1601	O	VAL	A	993	70.748	73.116	22.101	1.00	20.00
ATOM	1602	CB	VAL	A	993	72.102	70.746	20.159	1.00	20.00
ATOM	1603	CG1	VAL	A	993	71.570	69.843	21.226	1.00	20.00
ATOM	1604	CG2	VAL	A	993	71.121	70.843	19.076	1.00	20.00
ATOM	1606	N	LYS	A	994	70.990	74.076	20.082	1.00	20.00
ATOM	1607	CA	LYS	A	994	69.917	75.099	20.335	1.00	20.00
ATOM	1608	C	LYS	A	994	69.171	75.616	19.093	1.00	20.00
ATOM	1609	O	LYS	A	994	69.784	76.097	18.105	1.00	20.00
ATOM	1610	CB	LYS	A	994	70.508	76.336	21.083	1.00	20.00
ATOM	1611	CG	LYS	A	994	69.513	77.422	21.498	1.00	20.00
ATOM	1612	CD	LYS	A	994	69.827	78.812	20.847	1.00	20.00

FIG. 4W

ATOM	1613	CE	LYS	A	994	69.627	80.017	21.856	1.00	20.00
ATOM	1614	NZ	LYS	A	994	70.649	81.165	21.795	1.00	20.00
ATOM	1619	N	LYS	A	995	67.841	75.573	19.202	1.00	20.00
ATOM	1620	CA	LYS	A	995	66.914	75.962	18.132	1.00	20.00
ATOM	1621	C	LYS	A	995	65.884	74.827	18.184	1.00	20.00
ATOM	1622	O	LYS	A	995	65.303	74.470	17.139	1.00	20.00
ATOM	1623	CB	LYS	A	995	67.633	75.996	16.736	1.00	20.00
ATOM	1624	OXT	LYS	A	995	65.718	74.295	19.306	1.00	20.00
ATOM	1626	N	PRO	A	001	59.536	69.751	22.343	1.00	20.00
ATOM	1627	CA	PRO	A	001	60.339	69.285	23.473	1.00	20.00
ATOM	1628	C	PRO	A	001	60.137	70.032	24.772	1.00	20.00
ATOM	1629	O	PRO	A	001	60.361	69.470	25.821	1.00	20.00
ATOM	1630	CB	PRO	A	001	61.803	69.328	23.049	1.00	20.00
ATOM	1631	CG	PRO	A	001	61.735	69.311	21.525	1.00	20.00
ATOM	1632	CD	PRO	A	001	60.238	69.446	21.080	1.00	20.00
ATOM	1635	N	VAL	A	002	59.712	71.287	24.728	1.00	20.00
ATOM	1636	CA	VAL	A	002	59.503	72.082	25.958	1.00	20.00
ATOM	1637	C	VAL	A	002	58.748	71.338	27.019	1.00	20.00
ATOM	1638	O	VAL	A	002	58.868	71.595	28.206	1.00	20.00
ATOM	1639	CB	VAL	A	002	58.690	73.333	25.706	1.00	20.00
ATOM	1640	CG1	VAL	A	002	58.862	74.285	26.868	1.00	20.00
ATOM	1641	CG2	VAL	A	002	59.105	73.960	24.419	1.00	20.00
ATOM	1643	N	ARG	A	003	57.939	70.406	26.586	1.00	20.00
ATOM	1644	CA	ARG	A	003	57.158	69.637	27.519	1.00	20.00
ATOM	1645	C	ARG	A	003	57.966	68.497	28.085	1.00	20.00
ATOM	1646	O	ARG	A	003	57.686	68.013	29.163	1.00	20.00
ATOM	1647	CB	ARG	A	003	55.943	69.145	26.797	1.00	20.00
ATOM	1648	CG	ARG	A	003	55.600	70.041	25.655	1.00	20.00
ATOM	1649	CD	ARG	A	003	54.176	69.825	25.386	1.00	20.00
ATOM	1650	NE	ARG	A	003	53.404	70.556	26.347	1.00	20.00
ATOM	1651	CZ	ARG	A	003	52.340	71.236	25.991	1.00	20.00
ATOM	1652	NH1	ARG	A	003	52.002	71.218	24.710	1.00	20.00
ATOM	1653	NH2	ARG	A	003	51.653	71.922	26.889	1.00	20.00
ATOM	1660	N	TRP	A	004	58.998	68.136	27.340	1.00	20.00
ATOM	1661	CA	TRP	A	004	59.930	67.076	27.691	1.00	20.00
ATOM	1662	C	TRP	A	004	61.183	67.519	28.368	1.00	20.00
ATOM	1663	O	TRP	A	004	61.602	66.921	29.361	1.00	20.00
ATOM	1664	CB	TRP	A	004	60.293	66.257	26.452	1.00	20.00
ATOM	1665	CG	TRP	A	004	59.275	65.242	26.277	1.00	20.00
ATOM	1666	CD1	TRP	A	004	59.163	64.113	27.004	1.00	20.00
ATOM	1667	CD2	TRP	A	004	58.027	65.395	25.588	1.00	20.00
ATOM	1668	NE1	TRP	A	004	57.932	63.567	26.839	1.00	20.00
ATOM	1669	CE2	TRP	A	004	57.208	64.336	25.976	1.00	20.00
ATOM	1670	CE3	TRP	A	004	57.518	66.339	24.696	1.00	20.00
ATOM	1671	CZ2	TRP	A	004	55.911	64.185	25.506	1.00	20.00
ATOM	1672	CZ3	TRP	A	004	56.192	66.185	24.224	1.00	20.00
ATOM	1673	CH2	TRP	A	004	55.426	65.126	24.632	1.00	20.00
ATOM	1676	N	MET	A	005	61.767	68.590	27.874	1.00	20.00
ATOM	1677	CA	MET	A	005	63.025	69.060	28.428	1.00	20.00
ATOM	1678	C	MET	A	005	63.185	69.238	29.950	1.00	20.00
ATOM	1679	O	MET	A	005	62.268	69.013	30.733	1.00	20.00
ATOM	1680	CB	MET	A	005	63.433	70.335	27.699	1.00	20.00
ATOM	1681	CG	MET	A	005	64.246	70.052	26.452	1.00	20.00
ATOM	1682	SD	MET	A	005	63.856	71.198	25.171	1.00	20.00
ATOM	1683	CE	MET	A	005	64.138	72.700	26.081	1.00	20.00
ATOM	1685	N	ALA	A	006	64.402	69.581	30.358	1.00	20.00
ATOM	1686	CA	ALA	A	006	64.714	69.835	31.765	1.00	20.00

FIG. 4X

ATOM	1687	C	ALA	A	006	65.147	71.295	31.859	1.00 20.00
ATOM	1688	O	ALA	A	006	65.854	71.804	30.965	1.00 20.00
ATOM	1689	CB	ALA	A	006	65.819	68.944	32.215	1.00 20.00
ATOM	1691	N	ILE	A	007	64.694	71.961	32.930	1.00 20.00
ATOM	1692	CA	ILE	A	007	64.982	73.368	33.167	1.00 20.00
ATOM	1693	C	ILE	A	007	66.361	73.633	32.607	1.00 20.00
ATOM	1694	O	ILE	A	007	66.500	74.388	31.663	1.00 20.00
ATOM	1695	CB	ILE	A	007	64.876	73.725	34.674	1.00 20.00
ATOM	1696	CG1	ILE	A	007	65.897	72.943	35.501	1.00 20.00
ATOM	1697	CG2	ILE	A	007	63.518	73.339	35.193	1.00 20.00
ATOM	1698	CD1	ILE	A	007	66.781	73.773	36.516	1.00 20.00
ATOM	1700	N	GLU	A	008	67.361	72.921	33.131	1.00 20.00
ATOM	1701	CA	GLU	A	008	68.768	73.052	32.719	1.00 20.00
ATOM	1702	C	GLU	A	008	68.886	73.301	31.217	1.00 20.00
ATOM	1703	O	GLU	A	008	69.401	74.319	30.811	1.00 20.00
ATOM	1704	CB	GLU	A	008	69.565	71.799	33.174	1.00 20.00
ATOM	1705	CG	GLU	A	008	69.424	70.540	32.296	1.00 20.00
ATOM	1706	CD	GLU	A	008	69.290	69.267	33.131	1.00 20.00
ATOM	1707	OE1	GLU	A	008	69.605	69.369	34.325	1.00 20.00
ATOM	1708	OE2	GLU	A	008	68.867	68.187	32.613	1.00 20.00
ATOM	1710	N	SER	A	009	68.388	72.388	30.384	1.00 20.00
ATOM	1711	CA	SER	A	009	68.456	72.641	28.947	1.00 20.00
ATOM	1712	C	SER	A	009	67.387	73.630	28.440	1.00 20.00
ATOM	1713	O	SER	A	009	67.491	74.109	27.327	1.00 20.00
ATOM	1714	CB	SER	A	009	68.424	71.329	28.129	1.00 20.00
ATOM	1715	OG	SER	A	009	67.325	70.511	28.426	1.00 20.00
ATOM	1718	N	LEU	A	010	66.361	73.915	29.246	1.00 20.00
ATOM	1719	CA	LEU	A	010	65.328	74.909	28.869	1.00 20.00
ATOM	1720	C	LEU	A	010	66.043	76.294	28.797	1.00 20.00
ATOM	1721	O	LEU	A	010	65.881	77.047	27.816	1.00 20.00
ATOM	1722	CB	LEU	A	010	64.213	74.966	29.928	1.00 20.00
ATOM	1723	CG	LEU	A	010	62.880	74.229	29.760	1.00 20.00
ATOM	1724	CD1	LEU	A	010	61.863	75.034	30.483	1.00 20.00
ATOM	1725	CD2	LEU	A	010	62.459	74.066	28.330	1.00 20.00
ATOM	1727	N	ASN	A	011	66.825	76.577	29.854	1.00 20.00
ATOM	1728	CA	ASN	A	011	67.663	77.762	30.020	1.00 20.00
ATOM	1729	C	ASN	A	011	68.799	77.692	28.983	1.00 20.00
ATOM	1730	O	ASN	A	011	68.799	78.348	27.914	1.00 20.00
ATOM	1731	CB	ASN	A	011	68.303	77.725	31.386	1.00 20.00
ATOM	1732	CG	ASN	A	011	67.325	77.469	32.474	1.00 20.00
ATOM	1733	OD1	ASN	A	011	66.150	77.759	32.316	1.00 20.00
ATOM	1734	ND2	ASN	A	011	67.791	76.929	33.607	1.00 20.00
ATOM	1738	N	TYR	A	012	69.774	76.859	29.325	1.00 20.00
ATOM	1739	CA	TYR	A	012	70.918	76.611	28.481	1.00 20.00
ATOM	1740	C	TYR	A	012	70.488	75.487	27.544	1.00 20.00
ATOM	1741	O	TYR	A	012	69.908	74.499	28.020	1.00 20.00
ATOM	1742	CB	TYR	A	012	72.047	76.179	29.370	1.00 20.00
ATOM	1743	CG	TYR	A	012	71.787	76.590	30.784	1.00 20.00
ATOM	1744	CD1	TYR	A	012	71.854	75.680	31.809	1.00 20.00
ATOM	1745	CD2	TYR	A	012	71.474	77.879	31.097	1.00 20.00
ATOM	1746	CE1	TYR	A	012	71.619	76.047	33.097	1.00 20.00
ATOM	1747	CE2	TYR	A	012	71.246	78.242	32.357	1.00 20.00
ATOM	1748	CZ	TYR	A	012	71.321	77.328	33.361	1.00 20.00
ATOM	1749	OH	TYR	A	012	71.143	77.709	34.668	1.00 20.00
ATOM	1752	N	SER	A	013	70.711	75.615	26.235	1.00 20.00
ATOM	1753	CA	SER	A	013	70.309	74.544	25.335	1.00 20.00
ATOM	1754	C	SER	A	013	71.274	73.385	25.467	1.00 20.00

FIG. 4Y

ATOM	1755	O	SER	A	013	71.810	72.898	24.464	1.00 20.00
ATOM	1756	CB	SER	A	013	70.291	75.025	23.898	1.00 20.00
ATOM	1757	OG	SER	A	013	70.122	76.432	23.813	1.00 20.00
ATOM	1760	N	VAL	A	014	71.469	72.957	26.713	1.00 20.00
ATOM	1761	CA	VAL	A	014	72.378	71.890	27.084	1.00 20.00
ATOM	1762	C	VAL	A	014	71.711	70.603	27.571	1.00 20.00
ATOM	1763	O	VAL	A	014	70.895	70.613	28.493	1.00 20.00
ATOM	1764	CB	VAL	A	014	73.316	72.316	26.230	1.00 20.00
ATOM	1765	CG1	VAL	A	014	74.335	73.331	27.748	1.00 20.00
ATOM	1766	CG2	VAL	A	014	72.490	72.849	29.394	1.00 20.00
ATOM	1768	N	TYR	A	015	72.100	69.472	27.009	1.00 20.00
ATOM	1769	CA	TYR	A	015	71.502	68.235	27.446	1.00 20.00
ATOM	1770	C	TYR	A	015	72.543	67.266	28.029	1.00 20.00
ATOM	1771	O	TYR	A	015	73.619	67.072	27.494	1.00 20.00
ATOM	1772	CB	TYR	A	015	70.783	67.599	26.252	1.00 20.00
ATOM	1773	CG	TYR	A	015	69.875	68.533	25.477	1.00 20.00
ATOM	1774	CD1	TYR	A	015	70.194	68.918	24.179	1.00 20.00
ATOM	1775	CD2	TYR	A	015	68.665	68.975	26.022	1.00 20.00
ATOM	1776	CE1	TYR	A	015	69.334	69.718	23.416	1.00 20.00
ATOM	1777	CE2	TYR	A	015	67.782	69.778	25.286	1.00 20.00
ATOM	1778	CZ	TYR	A	015	68.116	70.150	23.968	1.00 20.00
ATOM	1779	OH	TYR	A	015	67.249	70.935	23.209	1.00 20.00
ATOM	1782	N	THR	A	016	72.253	66.679	29.161	1.00 20.00
ATOM	1783	CA	THR	A	016	73.172	65.695	29.673	1.00 20.00
ATOM	1784	C	THR	A	016	72.464	64.347	29.834	1.00 20.00
ATOM	1785	O	THR	A	016	71.573	63.995	29.086	1.00 20.00
ATOM	1786	CB	THR	A	016	73.717	66.097	31.000	1.00 20.00
ATOM	1787	OG1	THR	A	016	72.692	66.000	31.993	1.00 20.00
ATOM	1788	CG2	THR	A	016	74.253	67.455	30.909	1.00 20.00
ATOM	1791	N	THR	A	017	72.891	63.584	30.818	1.00 20.00
ATOM	1792	CA	THR	A	017	72.235	62.339	31.031	1.00 20.00
ATOM	1793	C	THR	A	017	71.021	62.785	31.819	1.00 20.00
ATOM	1794	O	THR	A	017	69.889	62.570	31.364	1.00 20.00
ATOM	1795	CB	THR	A	017	73.112	61.308	31.826	1.00 20.00
ATOM	1796	OG1	THR	A	017	73.546	60.286	30.931	1.00 20.00
ATOM	1797	CG2	THR	A	017	72.315	60.660	32.954	1.00 20.00
ATOM	1800	N	ASN	A	018	71.265	63.454	32.958	1.00 20.00
ATOM	1801	CA	ASN	A	018	70.189	63.934	33.825	1.00 20.00
ATOM	1802	C	ASN	A	018	69.025	64.568	33.108	1.00 20.00
ATOM	1803	O	ASN	A	018	67.937	64.530	33.636	1.00 20.00
ATOM	1804	CB	ASN	A	018	70.696	64.904	34.868	1.00 20.00
ATOM	1805	CG	ASN	A	018	71.785	64.331	35.676	1.00 20.00
ATOM	1806	OD1	ASN	A	018	71.761	64.412	36.887	1.00 20.00
ATOM	1807	ND2	ASN	A	018	72.767	63.734	35.013	1.00 20.00
ATOM	1811	N	SER	A	019	69.247	65.184	31.948	1.00 20.00
ATOM	1812	CA	SER	A	019	68.132	65.740	31.199	1.00 20.00
ATOM	1813	C	SER	A	019	67.362	64.513	30.704	1.00 20.00
ATOM	1814	O	SER	A	019	66.145	64.414	30.875	1.00 20.00
ATOM	1815	CB	SER	A	019	68.613	66.544	30.006	1.00 20.00
ATOM	1816	OG	SER	A	019	69.999	66.633	30.051	1.00 20.00
ATOM	1819	N	ASP	A	020	68.110	63.583	30.104	1.00 20.00
ATOM	1820	CA	ASP	A	020	67.596	62.309	29.604	1.00 20.00
ATOM	1821	C	ASP	A	020	66.784	61.679	30.741	1.00 20.00
ATOM	1822	O	ASP	A	020	65.672	61.194	30.543	1.00 20.00
ATOM	1823	CB	ASP	A	020	68.767	61.388	29.217	1.00 20.00
ATOM	1824	CG	ASP	A	020	69.154	61.484	27.729	1.00 20.00
ATOM	1825	OD1	ASP	A	020	68.649	62.363	26.979	1.00 20.00

FIG. 4Z

ATOM	1826	OD2	ASP	A	020	69.992	60.673	27.292	1.00	20.00
ATOM	1828	N	VAL	A	021	67.294	61.728	31.955	1.00	20.00
ATOM	1829	CA	VAL	A	021	66.522	61.083	32.960	1.00	20.00
ATOM	1830	C	VAL	A	021	65.300	61.826	33.326	1.00	20.00
ATOM	1831	O	VAL	A	021	64.372	61.212	33.879	1.00	20.00
ATOM	1832	CB	VAL	A	021	67.316	60.766	34.204	1.00	20.00
ATOM	1833	CG1	VAL	A	021	66.471	60.862	35.417	1.00	20.00
ATOM	1834	CG2	VAL	A	021	67.803	59.362	34.110	1.00	20.00
ATOM	1836	N	TRP	A	022	65.290	63.135	33.035	1.00	20.00
ATOM	1837	CA	TRP	A	022	64.157	64.016	33.326	1.00	20.00
ATOM	1838	C	TRP	A	022	63.051	63.699	32.319	1.00	20.00
ATOM	1839	O	TRP	A	022	61.948	63.268	32.629	1.00	20.00
ATOM	1840	CB	TRP	A	022	64.596	65.468	33.160	1.00	20.00
ATOM	1841	CG	TRP	A	022	63.439	66.467	33.254	1.00	20.00
ATOM	1842	CD1	TRP	A	022	62.437	66.648	32.337	1.00	20.00
ATOM	1843	CD2	TRP	A	022	63.161	67.366	34.322	1.00	20.00
ATOM	1844	NE1	TRP	A	022	61.576	67.578	32.767	1.00	20.00
ATOM	1845	CE2	TRP	A	022	61.985	68.049	33.984	1.00	20.00
ATOM	1846	CE3	TRP	A	022	63.791	67.662	35.529	1.00	20.00
ATOM	1847	CZ2	TRP	A	022	61.413	69.029	34.815	1.00	20.00
ATOM	1848	CZ3	TRP	A	022	63.237	68.626	36.355	1.00	20.00
ATOM	1849	CH2	TRP	A	022	62.052	69.303	35.992	1.00	20.00
ATOM	1852	N	SER	A	023	63.407	63.969	31.084	1.00	20.00
ATOM	1853	CA	SER	A	023	62.591	63.721	29.928	1.00	20.00
ATOM	1854	C	SER	A	023	61.978	62.316	30.007	1.00	20.00
ATOM	1855	O	SER	A	023	60.863	62.092	29.540	1.00	20.00
ATOM	1856	CB	SER	A	023	63.497	63.860	28.709	1.00	20.00
ATOM	1857	OG	SER	A	023	62.747	63.795	27.527	1.00	20.00
ATOM	1860	N	TYR	A	024	62.731	61.390	30.617	1.00	20.00
ATOM	1861	CA	TYR	A	024	62.361	59.980	30.801	1.00	20.00
ATOM	1862	C	TYR	A	024	60.980	59.761	31.454	1.00	20.00
ATOM	1863	O	TYR	A	024	60.137	58.991	30.967	1.00	20.00
ATOM	1864	CB	TYR	A	024	63.436	59.307	31.627	1.00	20.00
ATOM	1865	CG	TYR	A	024	63.129	57.866	31.859	1.00	20.00
ATOM	1866	CD1	TYR	A	024	63.276	56.948	30.849	1.00	20.00
ATOM	1867	CD2	TYR	A	024	62.479	57.473	33.019	1.00	20.00
ATOM	1868	CE1	TYR	A	024	62.766	55.706	30.979	1.00	20.00
ATOM	1869	CE2	TYR	A	024	61.962	56.236	33.157	1.00	20.00
ATOM	1870	CZ	TYR	A	024	62.099	55.365	32.135	1.00	20.00
ATOM	1871	OH	TYR	A	024	61.517	54.160	32.263	1.00	20.00
ATOM	1874	N	GLY	A	025	60.803	60.436	32.583	1.00	20.00
ATOM	1875	CA	GLY	A	025	59.558	60.427	33.311	1.00	20.00
ATOM	1876	C	GLY	A	025	58.477	61.257	32.614	1.00	20.00
ATOM	1877	O	GLY	A	025	57.365	61.290	33.058	1.00	20.00
ATOM	1879	N	VAL	A	026	58.747	61.974	31.544	1.00	20.00
ATOM	1880	CA	VAL	A	026	57.596	62.614	30.980	1.00	20.00
ATOM	1881	C	VAL	A	026	57.057	61.313	30.484	1.00	20.00
ATOM	1882	O	VAL	A	026	56.006	60.906	30.923	1.00	20.00
ATOM	1883	CB	VAL	A	026	57.889	63.625	29.823	1.00	20.00
ATOM	1884	CG1	VAL	A	026	56.583	64.258	29.328	1.00	20.00
ATOM	1885	CG2	VAL	A	026	58.746	64.717	30.327	1.00	20.00
ATOM	1887	N	LEU	A	027	57.843	60.639	29.632	1.00	20.00
ATOM	1888	CA	LEU	A	027	57.535	59.273	29.064	1.00	20.00
ATOM	1889	C	LEU	A	027	56.767	58.278	30.014	1.00	20.00
ATOM	1890	O	LEU	A	027	55.745	57.736	29.702	1.00	20.00
ATOM	1891	CB	LEU	A	027	58.852	58.615	28.663	1.00	20.00
ATOM	1892	CG	LEU	A	027	58.843	57.551	27.579	1.00	20.00

FIG. 4AA

ATOM	1893	CD1	LEU	A	027	58.238	58.171	26.367	1.00 20.00
ATOM	1894	CD2	LEU	A	027	60.239	57.031	27.287	1.00 20.00
ATOM	1896	N	LEU	A	028	57.333	58.031	31.171	1.00 20.00
ATOM	1897	CA	LEU	A	028	56.723	57.188	32.128	1.00 20.00
ATOM	1898	C	LEU	A	028	55.330	57.638	32.349	1.00 20.00
ATOM	1899	O	LEU	A	028	54.428	56.817	32.517	1.00 20.00
ATOM	1900	CB	LEU	A	028	57.455	57.281	33.427	1.00 20.00
ATOM	1901	CG	LEU	A	028	56.778	56.395	34.430	1.00 20.00
ATOM	1902	CD1	LEU	A	028	56.765	55.005	33.926	1.00 20.00
ATOM	1903	CD2	LEU	A	028	57.488	56.475	35.740	1.00 20.00
ATOM	1905	N	TRP	A	029	55.148	58.961	32.409	1.00 20.00
ATOM	1906	CA	TRP	A	029	53.820	59.578	32.612	1.00 20.00
ATOM	1907	C	TRP	A	029	53.028	59.464	31.295	1.00 20.00
ATOM	1908	O	TRP	A	029	51.869	59.142	31.301	1.00 20.00
ATOM	1909	CB	TRP	A	029	54.010	61.029	33.088	1.00 20.00
ATOM	1910	CG	TRP	A	029	52.746	61.841	33.293	1.00 20.00
ATOM	1911	CD1	TRP	A	029	52.207	62.275	34.483	1.00 20.00
ATOM	1912	CD2	TRP	A	029	51.934	62.381	32.271	1.00 20.00
ATOM	1913	NE1	TRP	A	029	51.113	63.057	34.241	1.00 20.00
ATOM	1914	CE2	TRP	A	029	50.925	63.138	32.892	1.00 20.00
ATOM	1915	CE3	TRP	A	029	51.962	62.298	30.886	1.00 20.00
ATOM	1916	CZ2	TRP	A	029	49.975	63.798	32.185	1.00 20.00
ATOM	1917	CZ3	TRP	A	029	51.018	62.951	30.186	1.00 20.00
ATOM	1918	CH2	TRP	A	029	50.030	63.701	30.830	1.00 20.00
ATOM	1921	N	GLU	A	030	53.684	59.695	30.166	1.00 20.00
ATOM	1922	CA	GLU	A	030	53.067	59.537	28.861	1.00 20.00
ATOM	1923	C	GLU	A	030	52.592	58.103	28.823	1.00 20.00
ATOM	1924	O	GLU	A	030	51.775	57.758	27.982	1.00 20.00
ATOM	1925	CB	GLU	A	030	54.099	59.616	27.737	1.00 20.00
ATOM	1926	CG	GLU	A	030	54.380	60.917	27.071	1.00 20.00
ATOM	1927	CD	GLU	A	030	55.162	60.706	25.771	1.00 20.00
ATOM	1928	OE1	GLU	A	030	55.818	59.668	25.665	1.00 20.00
ATOM	1929	OE2	GLU	A	030	55.144	61.535	24.838	1.00 20.00
ATOM	1931	N	ILE	A	031	53.124	57.260	29.711	1.00 20.00
ATOM	1932	CA	ILE	A	031	52.839	55.820	29.680	1.00 20.00
ATOM	1933	C	ILE	A	031	51.803	55.305	30.628	1.00 20.00
ATOM	1934	O	ILE	A	031	50.931	54.585	30.219	1.00 20.00
ATOM	1935	CB	ILE	A	031	54.192	54.974	29.833	1.00 20.00
ATOM	1936	CG1	ILE	A	031	54.803	54.722	28.459	1.00 20.00
ATOM	1937	CG2	ILE	A	031	53.964	53.607	30.495	1.00 20.00
ATOM	1938	CD1	ILE	A	031	56.144	54.104	28.543	1.00 20.00
ATOM	1940	N	VAL	A	032	51.893	55.672	31.892	1.00 20.00
ATOM	1941	CA	VAL	A	032	50.918	55.223	32.895	1.00 20.00
ATOM	1942	C	VAL	A	032	49.618	55.914	32.620	1.00 20.00
ATOM	1943	O	VAL	A	032	48.706	55.811	33.412	1.00 20.00
ATOM	1944	CB	VAL	A	032	51.306	55.664	34.327	1.00 20.00
ATOM	1945	CG1	VAL	A	032	50.610	56.932	34.667	1.00 20.00
ATOM	1946	CG2	VAL	A	032	50.962	54.602	35.333	1.00 20.00
ATOM	1948	N	SER	A	033	49.552	56.605	31.493	1.00 20.00
ATOM	1949	CA	SER	A	033	48.413	57.405	31.146	1.00 20.00
ATOM	1950	C	SER	A	033	47.776	57.027	29.850	1.00 20.00
ATOM	1951	O	SER	A	033	46.634	57.396	29.585	1.00 20.00
ATOM	1952	CB	SER	A	033	48.828	58.889	31.116	1.00 20.00
ATOM	1953	OG	SER	A	033	49.492	59.239	29.905	1.00 20.00
ATOM	1956	N	LEU	A	034	48.513	56.329	29.019	1.00 20.00
ATOM	1957	CA	LEU	A	034	47.975	55.904	27.758	1.00 20.00
ATOM	1958	C	LEU	A	034	47.939	57.037	26.801	1.00 20.00

FIG. 4BB

ATOM	1959	O	LEU	A	034	46.917	57.357	26.219	1.00 20.00
ATOM	1960	CB	LEU	A	034	46.580	55.366	27.923	1.00 20.00
ATOM	1961	CG	LEU	A	034	46.208	54.020	28.500	1.00 20.00
ATOM	1962	CD1	LEU	A	034	46.074	54.041	29.977	1.00 20.00
ATOM	1963	CD2	LEU	A	034	44.892	53.709	27.900	1.00 20.00
ATOM	1965	N	GLY	A	035	49.091	57.663	26.658	1.00 20.00
ATOM	1966	CA	GLY	A	035	49.248	58.759	25.715	1.00 20.00
ATOM	1967	C	GLY	A	035	48.581	60.112	25.920	1.00 20.00
ATOM	1968	O	GLY	A	035	48.145	60.734	24.947	1.00 20.00
ATOM	1970	N	GLY	A	036	48.511	60.580	27.156	1.00 20.00
ATOM	1971	CA	GLY	A	036	47.902	61.874	27.364	1.00 20.00
ATOM	1972	C	GLY	A	036	48.981	62.925	27.245	1.00 20.00
ATOM	1973	O	GLY	A	036	50.097	62.697	27.759	1.00 20.00
ATOM	1975	N	THR	A	037	48.692	64.027	26.543	1.00 20.00
ATOM	1976	CA	THR	A	037	49.656	65.126	26.400	1.00 20.00
ATOM	1977	C	THR	A	037	50.114	65.691	27.757	1.00 20.00
ATOM	1978	O	THR	A	037	49.289	65.966	28.616	1.00 20.00
ATOM	1979	CB	THR	A	037	49.038	66.308	25.664	1.00 20.00
ATOM	1980	OG1	THR	A	037	49.457	66.326	24.301	1.00 20.00
ATOM	1981	CG2	THR	A	037	49.447	67.597	26.327	1.00 20.00
ATOM	1984	N	PRO	A	038	51.445	65.866	27.966	1.00 20.00
ATOM	1985	CA	PRO	A	038	51.925	66.416	29.237	1.00 20.00
ATOM	1986	C	PRO	A	038	51.674	67.919	29.265	1.00 20.00
ATOM	1987	O	PRO	A	038	51.812	68.570	28.264	1.00 20.00
ATOM	1988	CB	PRO	A	038	53.401	66.083	29.223	1.00 20.00
ATOM	1989	CG	PRO	A	038	53.573	65.116	28.170	1.00 20.00
ATOM	1990	CD	PRO	A	038	52.592	65.497	27.134	1.00 20.00
ATOM	1991	N	TYR	A	039	51.296	68.471	30.407	1.00 20.00
ATOM	1992	CA	TYR	A	039	51.040	69.900	30.494	1.00 20.00
ATOM	1993	C	TYR	A	039	49.928	70.255	29.514	1.00 20.00
ATOM	1994	O	TYR	A	039	50.174	71.011	28.551	1.00 20.00
ATOM	1995	CB	TYR	A	039	52.317	70.678	30.156	1.00 20.00
ATOM	1996	CG	TYR	A	039	53.492	70.254	31.016	1.00 20.00
ATOM	1997	CD1	TYR	A	039	54.593	69.571	30.470	1.00 20.00
ATOM	1998	CD2	TYR	A	039	53.456	70.437	32.381	1.00 20.00
ATOM	1999	CE1	TYR	A	039	55.586	69.088	31.288	1.00 20.00
ATOM	2000	CE2	TYR	A	039	54.438	69.966	33.188	1.00 20.00
ATOM	2001	CZ	TYR	A	039	55.489	69.290	32.656	1.00 20.00
ATOM	2002	OH	TYR	A	039	56.405	68.759	33.532	1.00 20.00
ATOM	2005	N	CYS	A	040	48.713	69.706	29.757	1.00 20.00
ATOM	2006	CA	CYS	A	040	47.536	69.943	28.893	1.00 20.00
ATOM	2007	C	CYS	A	040	46.861	71.241	29.251	1.00 20.00
ATOM	2008	O	CYS	A	040	46.426	71.456	30.371	1.00 20.00
ATOM	2009	CB	CYS	A	040	46.518	68.779	28.952	1.00 20.00
ATOM	2010	SG	CYS	A	040	45.587	68.439	27.332	1.00 20.00
ATOM	2012	N	GLY	A	041	46.773	72.105	28.261	1.00 20.00
ATOM	2013	CA	GLY	A	041	46.197	73.417	28.496	1.00 20.00
ATOM	2014	C	GLY	A	041	47.251	74.257	29.222	1.00 20.00
ATOM	2015	O	GLY	A	041	46.977	74.928	30.241	1.00 20.00
ATOM	2017	N	MET	A	042	48.480	74.184	28.727	1.00 20.00
ATOM	2018	CA	MET	A	042	49.542	74.920	29.347	1.00 20.00
ATOM	2019	C	MET	A	042	50.391	75.508	28.241	1.00 20.00
ATOM	2020	O	MET	A	042	50.540	74.944	27.173	1.00 20.00
ATOM	2021	CB	MET	A	042	50.321	73.990	30.253	1.00 20.00
ATOM	2022	CG	MET	A	042	50.038	74.150	31.721	1.00 20.00
ATOM	2023	SD	MET	A	042	51.637	74.393	32.551	1.00 20.00
ATOM	2024	CE	MET	A	042	51.370	73.664	34.142	1.00 20.00

FIG. 4CC

ATOM	2026	N	THR	A	043	50.915	76.686	28.463	1.00 20.00
ATOM	2027	CA	THR	A	043	51.699	77.320	27.418	1.00 20.00
ATOM	2028	C	THR	A	043	53.137	77.204	27.856	1.00 20.00
ATOM	2029	O	THR	A	043	53.479	77.409	29.047	1.00 20.00
ATOM	2030	CB	THR	A	043	51.356	78.827	27.279	1.00 20.00
ATOM	2031	OG1	THR	A	043	51.534	79.465	28.565	1.00 20.00
ATOM	2032	CG2	THR	A	043	49.905	79.033	26.760	1.00 20.00
ATOM	2035	N	CYS	A	044	53.977	76.862	26.885	1.00 20.00
ATOM	2036	CA	CYS	A	044	55.388	76.714	27.139	1.00 20.00
ATOM	2037	C	CYS	A	044	55.681	77.866	28.075	1.00 20.00
ATOM	2038	O	CYS	A	044	55.836	77.638	29.269	1.00 20.00
ATOM	2039	CB	CYS	A	044	56.128	76.779	25.814	1.00 20.00
ATOM	2040	SG	CYS	A	044	55.373	75.549	24.616	1.00 20.00
ATOM	2042	N	ALA	A	045	55.664	79.092	27.554	1.00 20.00
ATOM	2043	CA	ALA	A	045	55.893	80.306	28.342	1.00 20.00
ATOM	2044	C	ALA	A	045	55.536	80.155	29.809	1.00 20.00
ATOM	2045	O	ALA	A	045	56.216	80.636	30.700	1.00 20.00
ATOM	2046	CB	ALA	A	045	55.082	81.416	27.760	1.00 20.00
ATOM	2048	N	GLU	A	046	54.429	79.482	30.050	1.00 20.00
ATOM	2049	CA	GLU	A	046	53.961	79.269	31.390	1.00 20.00
ATOM	2050	C	GLU	A	046	54.902	78.299	32.100	1.00 20.00
ATOM	2051	O	GLU	A	046	55.309	78.558	33.243	1.00 20.00
ATOM	2052	CB	GLU	A	046	52.556	78.738	31.281	1.00 20.00
ATOM	2053	CG	GLU	A	046	51.601	79.002	32.429	1.00 20.00
ATOM	2054	CD	GLU	A	046	50.437	78.036	32.341	1.00 20.00
ATOM	2055	OE1	GLU	A	046	50.182	77.380	33.378	1.00 20.00
ATOM	2056	OE2	GLU	A	046	49.814	77.940	31.222	1.00 20.00
ATOM	2058	N	LEU	A	047	55.251	77.192	31.437	1.00 20.00
ATOM	2059	CA	LEU	A	047	56.203	76.207	32.001	1.00 20.00
ATOM	2060	C	LEU	A	047	57.470	76.893	32.593	1.00 20.00
ATOM	2061	O	LEU	A	047	57.712	76.853	33.805	1.00 20.00
ATOM	2062	CB	LEU	A	047	56.639	75.203	30.914	1.00 20.00
ATOM	2063	CG	LEU	A	047	55.895	73.858	30.885	1.00 20.00
ATOM	2064	CD1	LEU	A	047	56.520	72.889	29.922	1.00 20.00
ATOM	2065	CD2	LEU	A	047	55.884	73.280	32.256	1.00 20.00
ATOM	2067	N	TYR	A	048	58.254	77.503	31.694	1.00 20.00
ATOM	2068	CA	TYR	A	048	59.483	78.267	31.974	1.00 20.00
ATOM	2069	C	TYR	A	048	59.499	78.978	33.311	1.00 20.00
ATOM	2070	O	TYR	A	048	60.325	78.669	34.188	1.00 20.00
ATOM	2071	CB	TYR	A	048	59.684	79.343	30.919	1.00 20.00
ATOM	2072	CG	TYR	A	048	60.217	78.874	29.611	1.00 20.00
ATOM	2073	CD1	TYR	A	048	59.370	78.692	28.518	1.00 20.00
ATOM	2074	CD2	TYR	A	048	61.570	78.629	29.459	1.00 20.00
ATOM	2075	CE1	TYR	A	048	59.868	78.263	27.278	1.00 20.00
ATOM	2076	CE2	TYR	A	048	62.094	78.206	28.248	1.00 20.00
ATOM	2077	CZ	TYR	A	048	61.250	78.013	27.141	1.00 20.00
ATOM	2078	OH	TYR	A	048	61.799	77.541	25.930	1.00 20.00
ATOM	2081	N	GLU	A	049	58.601	79.954	33.446	1.00 20.00
ATOM	2082	CA	GLU	A	049	58.527	80.725	34.680	1.00 20.00
ATOM	2083	C	GLU	A	049	58.074	79.756	35.720	1.00 20.00
ATOM	2084	O	GLU	A	049	58.417	79.886	36.903	1.00 20.00
ATOM	2085	CB	GLU	A	049	57.485	81.840	34.592	1.00 20.00
ATOM	2086	CG	GLU	A	049	57.233	82.519	35.947	1.00 20.00
ATOM	2087	CD	GLU	A	049	55.761	82.820	36.314	1.00 20.00
ATOM	2088	OE1	GLU	A	049	54.860	82.700	35.453	1.00 20.00
ATOM	2089	OE2	GLU	A	049	55.540	83.185	37.497	1.00 20.00
ATOM	2091	N	LYS	A	050	57.277	78.791	35.243	1.00 20.00

FIG. 4DD

ATOM	2092	CA	LYS	A	050	56.683	77.749	36.092	1.00 20.00
ATOM	2093	C	LYS	A	050	57.625	76.655	36.652	1.00 20.00
ATOM	2094	O	LYS	A	050	58.038	76.747	37.789	1.00 20.00
ATOM	2095	CB	LYS	A	050	55.465	77.116	35.362	1.00 20.00
ATOM	2097	N	LEU	A	051	57.965	75.640	35.880	1.00 20.00
ATOM	2098	CA	LEU	A	051	58.854	74.592	36.398	1.00 20.00
ATOM	2099	C	LEU	A	051	59.828	75.002	37.553	1.00 20.00
ATOM	2100	O	LEU	A	051	59.835	74.350	38.608	1.00 20.00
ATOM	2101	CB	LEU	A	051	59.655	73.957	35.239	1.00 20.00
ATOM	2102	CG	LEU	A	051	58.981	72.988	34.248	1.00 20.00
ATOM	2103	CD1	LEU	A	051	57.669	72.566	34.798	1.00 20.00
ATOM	2104	CD2	LEU	A	051	58.796	73.609	32.875	1.00 20.00
ATOM	2106	N	PRO	A	052	60.673	76.050	37.346	1.00 20.00
ATOM	2107	CA	PRO	A	052	61.652	76.601	38.292	1.00 20.00
ATOM	2108	C	PRO	A	052	61.323	76.418	39.750	1.00 20.00
ATOM	2109	O	PRO	A	052	61.675	75.396	40.337	1.00 20.00
ATOM	2110	CB	PRO	A	052	61.724	78.053	37.895	1.00 20.00
ATOM	2111	CG	PRO	A	052	61.556	78.008	36.389	1.00 20.00
ATOM	2112	CD	PRO	A	052	60.771	76.762	36.051	1.00 20.00
ATOM	2113	N	GLN	A	053	60.706	77.399	40.394	1.00 20.00
ATOM	2114	CA	GLN	A	053	60.319	77.126	41.783	1.00 20.00
ATOM	2115	C	GLN	A	053	58.915	76.531	41.498	1.00 20.00
ATOM	2116	O	GLN	A	053	58.116	76.198	42.386	1.00 20.00
ATOM	2117	CB	GLN	A	053	60.274	78.414	42.664	1.00 20.00
ATOM	2119	N	GLY	A	054	58.649	76.413	40.208	1.00 20.00
ATOM	2120	CA	GLY	A	054	57.454	75.745	39.784	1.00 20.00
ATOM	2121	C	GLY	A	054	57.520	74.261	40.190	1.00 20.00
ATOM	2122	O	GLY	A	054	58.564	73.730	40.654	1.00 20.00
ATOM	2124	N	TYR	A	055	56.363	73.629	40.002	1.00 20.00
ATOM	2125	CA	TYR	A	055	56.081	72.268	40.370	1.00 20.00
ATOM	2126	C	TYR	A	055	56.216	71.476	39.095	1.00 20.00
ATOM	2127	O	TYR	A	055	56.762	72.008	38.153	1.00 20.00
ATOM	2128	CB	TYR	A	055	54.647	72.256	40.889	1.00 20.00
ATOM	2129	CG	TYR	A	055	53.604	72.330	39.754	1.00 20.00
ATOM	2130	CD1	TYR	A	055	52.634	71.309	39.604	1.00 20.00
ATOM	2131	CD2	TYR	A	055	53.685	73.316	38.749	1.00 20.00
ATOM	2132	CE1	TYR	A	055	51.805	71.283	38.478	1.00 20.00
ATOM	2133	CE2	TYR	A	055	52.863	73.280	37.642	1.00 20.00
ATOM	2134	CZ	TYR	A	055	51.928	72.264	37.501	1.00 20.00
ATOM	2135	OH	TYR	A	055	51.114	72.171	36.375	1.00 20.00
ATOM	2138	N	ARG	A	056	55.738	70.232	39.048	1.00 20.00
ATOM	2139	CA	ARG	A	056	55.828	69.422	37.821	1.00 20.00
ATOM	2140	C	ARG	A	056	54.504	68.699	37.494	1.00 20.00
ATOM	2141	O	ARG	A	056	53.471	69.052	38.098	1.00 20.00
ATOM	2142	CB	ARG	A	056	56.926	68.379	37.948	1.00 20.00
ATOM	2143	CG	ARG	A	056	57.175	67.962	39.357	1.00 20.00
ATOM	2144	CD	ARG	A	056	58.538	68.505	39.833	1.00 20.00
ATOM	2145	NE	ARG	A	056	59.319	69.142	38.760	1.00 20.00
ATOM	2146	CZ	ARG	A	056	60.182	70.114	38.982	1.00 20.00
ATOM	2147	NH1	ARG	A	056	60.367	70.542	40.201	1.00 20.00
ATOM	2148	NH2	ARG	A	056	60.839	70.655	37.996	1.00 20.00
ATOM	2155	N	LEU	A	057	54.531	67.705	36.565	1.00 20.00
ATOM	2156	CA	LEU	A	057	53.312	66.955	36.203	1.00 20.00
ATOM	2157	C	LEU	A	057	52.643	66.257	37.370	1.00 20.00
ATOM	2158	O	LEU	A	057	53.221	65.587	38.191	1.00 20.00
ATOM	2159	CB	LEU	A	057	53.519	65.955	35.071	1.00 20.00
ATOM	2160	CG	LEU	A	057	53.850	66.384	33.632	1.00 20.00

FIG. 4EE

ATOM	2161	CD1	LEU	A	057	54.504	65.224	32.920	1.00 20.00
ATOM	2162	CD2	LEU	A	057	52.669	66.811	32.830	1.00 20.00
ATOM	2164	N	GLU	A	058	51.357	66.515	37.390	1.00 20.00
ATOM	2165	CA	GLU	A	058	50.325	66.093	38.333	1.00 20.00
ATOM	2166	C	GLU	A	058	50.078	64.562	38.297	1.00 20.00
ATOM	2167	O	GLU	A	058	50.013	63.978	37.216	1.00 20.00
ATOM	2168	CB	GLU	A	058	49.091	66.872	37.885	1.00 20.00
ATOM	2169	CG	GLU	A	058	48.798	66.637	36.334	1.00 20.00
ATOM	2170	CD	GLU	A	058	49.565	67.548	35.341	1.00 20.00
ATOM	2171	OE1	GLU	A	058	50.058	68.604	35.777	1.00 20.00
ATOM	2172	OE2	GLU	A	058	49.657	67.227	34.128	1.00 20.00
ATOM	2174	N	LYS	A	059	49.906	63.915	39.448	1.00 20.00
ATOM	2175	CA	LYS	A	059	49.693	62.458	39.420	1.00 20.00
ATOM	2176	C	LYS	A	059	48.502	61.929	38.655	1.00 20.00
ATOM	2177	O	LYS	A	059	47.366	62.213	38.971	1.00 20.00
ATOM	2178	CB	LYS	A	059	49.607	61.825	40.814	1.00 20.00
ATOM	2179	CG	LYS	A	059	49.383	60.289	40.717	1.00 20.00
ATOM	2180	CD	LYS	A	059	49.519	59.551	42.056	1.00 20.00
ATOM	2181	CE	LYS	A	059	48.286	59.754	42.979	1.00 20.00
ATOM	2182	NZ	LYS	A	059	47.400	58.540	43.161	1.00 20.00
ATOM	2187	N	PRO	A	060	48.753	61.095	37.662	1.00 20.00
ATOM	2188	CA	PRO	A	060	47.615	60.576	36.931	1.00 20.00
ATOM	2189	C	PRO	A	060	46.646	59.848	37.873	1.00 20.00
ATOM	2190	O	PRO	A	060	47.048	59.234	38.860	1.00 20.00
ATOM	2191	CB	PRO	A	060	48.260	59.643	35.923	1.00 20.00
ATOM	2192	CG	PRO	A	060	49.662	60.187	35.751	1.00 20.00
ATOM	2193	CD	PRO	A	060	50.018	60.555	37.147	1.00 20.00
ATOM	2194	N	LEU	A	061	45.371	59.984	37.543	1.00 20.00
ATOM	2195	CA	LEU	A	061	44.236	59.426	38.245	1.00 20.00
ATOM	2196	C	LEU	A	061	44.496	58.098	38.924	1.00 20.00
ATOM	2197	O	LEU	A	061	44.187	57.890	40.123	1.00 20.00
ATOM	2198	CB	LEU	A	061	43.055	59.243	37.248	1.00 20.00
ATOM	2199	CG	LEU	A	061	42.994	59.507	35.690	1.00 20.00
ATOM	2200	CD1	LEU	A	061	44.393	59.876	35.050	1.00 20.00
ATOM	2201	CD2	LEU	A	061	42.384	58.237	35.000	1.00 20.00
ATOM	2203	N	ASN	A	062	45.075	57.203	38.117	1.00 20.00
ATOM	2204	CA	ASN	A	062	45.378	55.820	38.502	1.00 20.00
ATOM	2205	C	ASN	A	062	46.840	55.286	38.537	1.00 20.00
ATOM	2206	O	ASN	A	062	47.079	54.209	37.999	1.00 20.00
ATOM	2207	CB	ASN	A	062	44.591	54.958	37.559	1.00 20.00
ATOM	2208	CG	ASN	A	062	44.675	55.478	36.220	1.00 20.00
ATOM	2209	OD1	ASN	A	062	45.731	55.960	35.816	1.00 20.00
ATOM	2210	ND2	ASN	A	062	43.590	55.443	35.504	1.00 20.00
ATOM	2214	N	CYS	A	063	47.812	56.005	39.100	1.00 20.00
ATOM	2215	CA	CYS	A	063	49.165	55.418	39.205	1.00 20.00
ATOM	2216	C	CYS	A	063	49.155	55.124	40.645	1.00 20.00
ATOM	2217	O	CYS	A	063	48.285	55.550	41.377	1.00 20.00
ATOM	2218	CB	CYS	A	063	50.364	56.362	39.046	1.00 20.00
ATOM	2219	SG	CYS	A	063	50.817	56.807	37.453	1.00 20.00
ATOM	2221	N	ASP	A	064	50.186	54.449	41.067	1.00 20.00
ATOM	2222	CA	ASP	A	064	50.291	54.106	42.448	1.00 20.00
ATOM	2223	C	ASP	A	064	51.455	54.945	42.917	1.00 20.00
ATOM	2224	O	ASP	A	064	52.521	54.903	42.319	1.00 20.00
ATOM	2225	CB	ASP	A	064	50.558	52.601	42.552	1.00 20.00
ATOM	2226	CG	ASP	A	064	50.951	52.180	43.945	1.00 20.00
ATOM	2227	OD1	ASP	A	064	50.078	51.628	44.664	1.00 20.00
ATOM	2228	OD2	ASP	A	064	52.131	52.394	44.309	1.00 20.00

FIG. 4FF

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ATOM	2230	N	ASP	A	065	51.259	55.718	43.973	1.00	20.00
ATOM	2231	CA	ASP	A	065	52.332	56.577	44.460	1.00	20.00
ATOM	2232	C	ASP	A	065	53.733	56.051	44.341	1.00	20.00
ATOM	2233	O	ASP	A	065	54.642	56.860	44.332	1.00	20.00
ATOM	2234	CB	ASP	A	065	52.062	57.029	45.875	1.00	20.00
ATOM	2235	CG	ASP	A	065	50.937	58.020	45.923	1.00	20.00
ATOM	2236	OD1	ASP	A	065	50.842	58.814	44.958	1.00	20.00
ATOM	2237	OD2	ASP	A	065	50.136	58.013	46.883	1.00	20.00
ATOM	2239	N	GLU	A	066	53.918	54.734	44.222	1.00	20.00
ATOM	2240	CA	GLU	A	066	55.255	54.179	44.049	1.00	20.00
ATOM	2241	C	GLU	A	066	55.670	54.466	42.600	1.00	20.00
ATOM	2242	O	GLU	A	066	56.854	54.554	42.311	1.00	20.00
ATOM	2243	CB	GLU	A	066	55.315	52.656	44.363	1.00	20.00
ATOM	2244	CG	GLU	A	066	54.520	52.182	45.635	1.00	20.00
ATOM	2245	CD	GLU	A	066	54.944	50.804	46.237	1.00	20.00
ATOM	2246	OE1	GLU	A	066	54.716	50.604	47.469	1.00	20.00
ATOM	2247	OE2	GLU	A	066	55.494	49.937	45.496	1.00	20.00
ATOM	2249	N	VAL	A	067	54.726	54.592	41.671	1.00	20.00
ATOM	2250	CA	VAL	A	067	55.092	54.941	40.293	1.00	20.00
ATOM	2251	C	VAL	A	067	55.224	56.462	40.180	1.00	20.00
ATOM	2252	O	VAL	A	067	56.000	56.986	39.410	1.00	20.00
ATOM	2253	CB	VAL	A	067	54.055	54.487	39.279	1.00	20.00
ATOM	2254	CG1	VAL	A	067	54.600	54.593	37.857	1.00	20.00
ATOM	2255	CG2	VAL	A	067	53.657	53.116	39.597	1.00	20.00
ATOM	2257	N	TYR	A	068	54.460	57.189	40.948	1.00	20.00
ATOM	2258	CA	TYR	A	068	54.614	58.609	40.861	1.00	20.00
ATOM	2259	C	TYR	A	068	55.973	59.018	41.455	1.00	20.00
ATOM	2260	O	TYR	A	068	56.712	59.819	40.831	1.00	20.00
ATOM	2261	CB	TYR	A	068	53.489	59.313	41.595	1.00	20.00
ATOM	2262	CG	TYR	A	068	53.361	60.752	41.220	1.00	20.00
ATOM	2263	CD1	TYR	A	068	53.128	61.124	39.920	1.00	20.00
ATOM	2264	CD2	TYR	A	068	53.490	61.746	42.186	1.00	20.00
ATOM	2265	CE1	TYR	A	068	53.031	62.478	39.603	1.00	20.00
ATOM	2266	CE2	TYR	A	068	53.395	63.060	41.887	1.00	20.00
ATOM	2267	CZ	TYR	A	068	53.171	63.435	40.612	1.00	20.00
ATOM	2268	OH	TYR	A	068	53.121	64.768	40.328	1.00	20.00
ATOM	2271	N	ASP	A	069	56.315	58.503	42.647	1.00	20.00
ATOM	2272	CA	ASP	A	069	57.609	58.859	43.214	1.00	20.00
ATOM	2273	C	ASP	A	069	58.773	58.615	42.263	1.00	20.00
ATOM	2274	O	ASP	A	069	59.744	59.344	42.299	1.00	20.00
ATOM	2275	CB	ASP	A	069	57.969	58.107	44.464	1.00	20.00
ATOM	2276	CG	ASP	A	069	59.422	58.423	44.879	1.00	20.00
ATOM	2277	OD1	ASP	A	069	60.352	57.615	44.540	1.00	20.00
ATOM	2278	OD2	ASP	A	069	59.635	59.510	45.509	1.00	20.00
ATOM	2280	N	LEU	A	070	58.720	57.565	41.452	1.00	20.00
ATOM	2281	CA	LEU	A	070	59.809	57.334	40.528	1.00	20.00
ATOM	2282	C	LEU	A	070	59.790	58.516	39.558	1.00	20.00
ATOM	2283	O	LEU	A	070	60.802	59.127	39.276	1.00	20.00
ATOM	2284	CB	LEU	A	070	59.609	56.013	39.765	1.00	20.00
ATOM	2285	CG	LEU	A	070	60.747	55.706	38.780	1.00	20.00
ATOM	2286	CD1	LEU	A	070	61.879	55.168	39.574	1.00	20.00
ATOM	2287	CD2	LEU	A	070	60.351	54.769	37.681	1.00	20.00
ATOM	2289	N	MET	A	071	58.597	58.816	39.073	1.00	20.00
ATOM	2290	CA	MET	A	071	58.336	59.892	38.116	1.00	20.00
ATOM	2291	C	MET	A	071	59.004	61.168	38.549	1.00	20.00
ATOM	2292	O	MET	A	071	59.698	61.796	37.776	1.00	20.00
ATOM	2293	CB	MET	A	071	56.818	60.169	38.000	1.00	20.00

FIG. 4GG

ATOM	2294	CG	MET	A	071	56.219	59.904	36.636	1.00 20.00
ATOM	2295	SD	MET	A	071	54.409	59.761	36.764	1.00 20.00
ATOM	2296	CE	MET	A	071	53.977	58.683	35.467	1.00 20.00
ATOM	2298	N	ARG	A	072	58.797	61.527	39.803	1.00 20.00
ATOM	2299	CA	ARG	A	072	59.303	62.762	40.345	1.00 20.00
ATOM	2300	C	ARG	A	072	60.739	62.807	40.778	1.00 20.00
ATOM	2301	O	ARG	A	072	61.312	63.884	40.945	1.00 20.00
ATOM	2302	CB	ARG	A	072	58.412	63.145	41.499	1.00 20.00
ATOM	2303	CG	ARG	A	072	56.978	63.140	41.074	1.00 20.00
ATOM	2304	CD	ARG	A	072	56.500	64.539	41.064	1.00 20.00
ATOM	2305	NE	ARG	A	072	56.642	65.063	42.415	1.00 20.00
ATOM	2306	CZ	ARG	A	072	56.484	66.337	42.720	1.00 20.00
ATOM	2307	NH1	ARG	A	072	56.181	67.175	41.753	1.00 20.00
ATOM	2308	NH2	ARG	A	072	56.642	66.771	43.968	1.00 20.00
ATOM	2315	N	GLN	A	073	61.325	61.647	41.011	1.00 20.00
ATOM	2316	CA	GLN	A	073	62.717	61.652	41.387	1.00 20.00
ATOM	2317	C	GLN	A	073	63.481	61.931	40.084	1.00 20.00
ATOM	2318	O	GLN	A	073	64.658	62.267	40.105	1.00 20.00
ATOM	2319	CB	GLN	A	073	63.124	60.316	41.973	1.00 20.00
ATOM	2320	CG	GLN	A	073	63.076	60.211	43.490	1.00 20.00
ATOM	2321	CD	GLN	A	073	63.603	58.852	43.962	1.00 20.00
ATOM	2322	OE1	GLN	A	073	63.853	58.641	45.159	1.00 20.00
ATOM	2323	NE2	GLN	A	073	63.792	57.925	43.008	1.00 20.00
ATOM	2327	N	CYS	A	074	62.819	61.805	38.947	1.00 20.00
ATOM	2328	CA	CYS	A	074	63.503	62.093	37.720	1.00 20.00
ATOM	2329	C	CYS	A	074	63.403	63.601	37.500	1.00 20.00
ATOM	2330	O	CYS	A	074	64.073	64.148	36.642	1.00 20.00
ATOM	2331	CB	CYS	A	074	62.847	61.361	36.524	1.00 20.00
ATOM	2332	SG	CYS	A	074	62.746	59.548	36.564	1.00 20.00
ATOM	2334	N	TRP	A	075	62.555	64.268	38.277	1.00 20.00
ATOM	2335	CA	TRP	A	075	62.311	65.708	38.110	1.00 20.00
ATOM	2336	C	TRP	A	075	62.906	66.552	39.231	1.00 20.00
ATOM	2337	O	TRP	A	075	62.503	67.692	39.466	1.00 20.00
ATOM	2338	CB	TRP	A	075	60.797	65.977	38.037	1.00 20.00
ATOM	2339	CG	TRP	A	075	60.090	65.403	36.830	1.00 20.00
ATOM	2340	CD1	TRP	A	075	60.586	65.308	35.565	1.00 20.00
ATOM	2341	CD2	TRP	A	075	58.768	64.834	36.789	1.00 20.00
ATOM	2342	NE1	TRP	A	075	59.669	64.720	34.751	1.00 20.00
ATOM	2343	CE2	TRP	A	075	58.542	64.416	35.468	1.00 20.00
ATOM	2344	CE3	TRP	A	075	57.755	64.634	37.742	1.00 20.00
ATOM	2345	CZ2	TRP	A	075	57.343	63.808	35.062	1.00 20.00
ATOM	2346	CZ3	TRP	A	075	56.551	64.024	37.331	1.00 20.00
ATOM	2347	CH2	TRP	A	075	56.366	63.624	36.002	1.00 20.00
ATOM	2350	N	ARG	A	076	63.865	65.959	39.934	1.00 20.00
ATOM	2351	CA	ARG	A	076	64.533	66.625	41.024	1.00 20.00
ATOM	2352	C	ARG	A	076	65.304	67.793	40.364	1.00 20.00
ATOM	2353	O	ARG	A	076	65.983	67.586	39.347	1.00 20.00
ATOM	2354	CB	ARG	A	076	65.462	65.607	41.699	1.00 20.00
ATOM	2355	CG	ARG	A	076	64.890	64.932	42.981	1.00 20.00
ATOM	2356	CD	ARG	A	076	65.230	63.413	43.072	1.00 20.00
ATOM	2357	NE	ARG	A	076	64.997	62.813	44.416	1.00 20.00
ATOM	2358	CZ	ARG	A	076	65.490	61.630	44.835	1.00 20.00
ATOM	2359	NH1	ARG	A	076	66.258	60.880	44.037	1.00 20.00
ATOM	2360	NH2	ARG	A	076	65.231	61.211	46.069	1.00 20.00
ATOM	2367	N	GLU	A	077	65.178	69.014	40.895	1.00 20.00
ATOM	2368	CA	GLU	A	077	65.885	70.155	40.318	1.00 20.00
ATOM	2369	C	GLU	A	077	67.310	69.773	39.983	1.00 20.00

FIG. 4HH

ATOM	2376	O	GLU	A	077	67.613	69.364	38.878	1.00	20.00
ATOM	2377	CB	GLU	A	077	65.889	71.343	41.278	1.00	20.00
ATOM	2373	N	LYS	A	078	68.184	69.910	40.953	1.00	20.00
ATOM	2374	CA	LYS	A	078	69.573	69.583	40.764	1.00	20.00
ATOM	2375	C	LYS	A	078	69.811	68.228	40.037	1.00	20.00
ATOM	2376	O	LYS	A	078	69.850	67.194	40.664	1.00	20.00
ATOM	2377	CB	LYS	A	078	70.225	69.573	42.138	1.00	20.00
ATOM	2378	CG	LYS	A	078	69.346	70.070	43.275	1.00	20.00
ATOM	2379	CD	LYS	A	078	70.069	69.962	44.591	1.00	20.00
ATOM	2380	CE	LYS	A	078	69.301	70.580	45.713	1.00	20.00
ATOM	2381	NZ	LYS	A	078	69.362	69.789	47.005	1.00	20.00
ATOM	2386	N	PRO	A	079	70.050	68.234	38.721	1.00	20.00
ATOM	2387	CA	PRO	A	079	70.261	66.980	38.006	1.00	20.00
ATOM	2388	C	PRO	A	079	70.943	65.885	38.771	1.00	20.00
ATOM	2389	O	PRO	A	079	70.451	64.770	38.811	1.00	20.00
ATOM	2390	CB	PRO	A	079	71.059	67.370	36.772	1.00	20.00
ATOM	2391	CG	PRO	A	079	70.896	68.782	36.633	1.00	20.00
ATOM	2392	CD	PRO	A	079	70.218	69.385	37.832	1.00	20.00
ATOM	2393	N	TYR	A	080	72.085	66.172	39.382	1.00	20.00
ATOM	2394	CA	TYR	A	080	72.804	65.132	40.133	1.00	20.00
ATOM	2395	C	TYR	A	080	71.975	64.531	41.286	1.00	20.00
ATOM	2396	O	TYR	A	080	72.444	63.680	42.014	1.00	20.00
ATOM	2397	CB	TYR	A	080	74.139	65.707	40.640	1.00	20.00
ATOM	2398	CG	TYR	A	080	74.006	66.804	41.677	1.00	20.00
ATOM	2399	CD1	TYR	A	080	74.086	66.521	43.022	1.00	20.00
ATOM	2400	CD2	TYR	A	080	73.757	68.117	41.304	1.00	20.00
ATOM	2401	CE1	TYR	A	080	73.915	67.500	43.955	1.00	20.00
ATOM	2402	CE2	TYR	A	080	73.588	69.104	42.245	1.00	20.00
ATOM	2403	CZ	TYR	A	080	73.664	68.784	43.562	1.00	20.00
ATOM	2404	OH	TYR	A	080	73.475	69.749	44.512	1.00	20.00
ATOM	2407	N	GLU	A	081	70.743	65.007	41.436	1.00	20.00
ATOM	2408	CA	GLU	A	081	69.817	64.540	42.462	1.00	20.00
ATOM	2409	C	GLU	A	081	68.878	63.538	41.797	1.00	20.00
ATOM	2410	O	GLU	A	081	68.205	62.751	42.451	1.00	20.00
ATOM	2411	CB	GLU	A	081	69.025	65.709	43.038	1.00	20.00
ATOM	2412	CG	GLU	A	081	69.358	66.053	44.505	1.00	20.00
ATOM	2413	CD	GLU	A	081	68.385	67.067	45.106	1.00	20.00
ATOM	2414	OE1	GLU	A	081	68.518	67.413	46.316	1.00	20.00
ATOM	2415	OE2	GLU	A	081	67.485	67.510	44.342	1.00	20.00
ATOM	2417	N	ARG	A	082	68.875	63.582	40.471	1.00	20.00
ATOM	2418	CA	ARG	A	082	68.097	62.678	39.655	1.00	20.00
ATOM	2419	C	ARG	A	082	68.622	61.223	39.710	1.00	20.00
ATOM	2420	O	ARG	A	082	69.814	60.963	39.981	1.00	20.00
ATOM	2421	CB	ARG	A	082	68.085	63.174	38.218	1.00	20.00
ATOM	2422	CG	ARG	A	082	66.784	63.856	37.837	1.00	20.00
ATOM	2423	CD	ARG	A	082	66.836	65.398	37.781	1.00	20.00
ATOM	2424	NE	ARG	A	082	67.235	65.908	36.451	1.00	20.00
ATOM	2425	CZ	ARG	A	082	67.427	67.194	36.163	1.00	20.00
ATOM	2426	NH1	ARG	A	082	67.258	68.107	37.101	1.00	20.00
ATOM	2427	NH2	ARG	A	082	67.805	67.552	34.947	1.00	20.00
ATOM	2434	N	PRO	A	083	67.725	60.237	39.513	1.00	20.00
ATOM	2435	CA	PRO	A	083	68.223	58.866	39.554	1.00	20.00
ATOM	2436	C	PRO	A	083	69.042	58.596	38.310	1.00	20.00
ATOM	2437	O	PRO	A	083	69.594	59.505	37.688	1.00	20.00
ATOM	2438	CB	PRO	A	083	66.942	58.037	39.582	1.00	20.00
ATOM	2439	CG	PRO	A	083	65.877	58.981	40.016	1.00	20.00
ATOM	2440	CD	PRO	A	083	66.265	60.243	39.330	1.00	20.00

FIG. 4II

ATOM	2441	N	SER	A	084	69.110	57.327	37.952	1.00 20.00
ATOM	2442	CA	SER	A	084	69.825	56.896	36.760	1.00 20.00
ATOM	2443	C	SER	A	084	69.131	55.647	36.225	1.00 20.00
ATOM	2444	O	SER	A	084	68.707	54.760	36.990	1.00 20.00
ATOM	2445	CB	SER	A	084	71.283	56.583	37.087	1.00 20.00
ATOM	2446	OG	SER	A	084	71.397	55.714	38.182	1.00 20.00
ATOM	2449	N	PHE	A	085	69.014	55.585	34.905	1.00 20.00
ATOM	2450	CA	PHE	A	085	68.378	54.457	34.249	1.00 20.00
ATOM	2451	C	PHE	A	085	68.808	53.087	34.761	1.00 20.00
ATOM	2452	O	PHE	A	085	68.185	52.089	34.478	1.00 20.00
ATOM	2453	CB	PHE	A	085	68.633	54.555	32.762	1.00 20.00
ATOM	2454	CG	PHE	A	085	68.121	55.805	32.170	1.00 20.00
ATOM	2455	CD1	PHE	A	085	68.888	56.546	31.303	1.00 20.00
ATOM	2456	CD2	PHE	A	085	66.866	56.277	32.507	1.00 20.00
ATOM	2457	CE1	PHE	A	085	68.402	57.738	30.784	1.00 20.00
ATOM	2458	CE2	PHE	A	085	66.395	57.456	31.995	1.00 20.00
ATOM	2459	CZ	PHE	A	085	67.160	58.174	31.140	1.00 20.00
ATOM	2461	N	ALA	A	086	69.890	53.030	35.509	1.00 20.00
ATOM	2462	CA	ALA	A	086	70.327	51.757	35.993	1.00 20.00
ATOM	2463	C	ALA	A	086	69.505	51.422	37.206	1.00 20.00
ATOM	2464	O	ALA	A	086	69.064	50.291	37.352	1.00 20.00
ATOM	2465	CB	ALA	A	086	71.777	51.807	36.323	1.00 20.00
ATOM	2467	N	GLN	A	087	69.266	52.398	38.071	1.00 20.00
ATOM	2468	CA	GLN	A	087	68.494	52.121	39.266	1.00 20.00
ATOM	2469	C	GLN	A	087	66.956	52.163	39.068	1.00 20.00
ATOM	2470	O	GLN	A	087	66.195	51.560	39.846	1.00 20.00
ATOM	2471	CB	GLN	A	087	68.936	53.074	40.388	1.00 20.00
ATOM	2472	CG	GLN	A	087	69.565	54.391	39.973	1.00 20.00
ATOM	2473	CD	GLN	A	087	70.381	55.057	41.121	1.00 20.00
ATOM	2474	OE1	GLN	A	087	71.123	56.032	40.897	1.00 20.00
ATOM	2475	NE2	GLN	A	087	70.244	54.536	42.341	1.00 20.00
ATOM	2479	N	ILE	A	088	66.533	52.883	38.025	1.00 20.00
ATOM	2480	CA	ILE	A	088	65.126	53.054	37.686	1.00 20.00
ATOM	2481	C	ILE	A	088	64.687	51.697	37.241	1.00 20.00
ATOM	2482	O	ILE	A	088	63.649	51.196	37.639	1.00 20.00
ATOM	2483	CB	ILE	A	088	64.938	54.057	36.496	1.00 20.00
ATOM	2484	CG1	ILE	A	088	64.769	55.490	37.007	1.00 20.00
ATOM	2485	CG2	ILE	A	088	63.729	53.684	35.655	1.00 20.00
ATOM	2486	CD1	ILE	A	088	65.373	56.556	36.035	1.00 20.00
ATOM	2488	N	LEU	A	089	65.515	51.128	36.379	1.00 20.00
ATOM	2489	CA	LEU	A	089	65.313	49.789	35.843	1.00 20.00
ATOM	2490	C	LEU	A	089	65.060	48.826	36.994	1.00 20.00
ATOM	2491	O	LEU	A	089	64.018	48.175	37.061	1.00 20.00
ATOM	2492	CB	LEU	A	089	66.540	49.336	35.092	1.00 20.00
ATOM	2493	CG	LEU	A	089	66.547	47.848	34.823	1.00 20.00
ATOM	2494	CD1	LEU	A	089	65.147	47.379	34.407	1.00 20.00
ATOM	2495	CD2	LEU	A	089	67.545	47.575	33.708	1.00 20.00
ATOM	2497	N	VAL	A	090	66.004	48.748	37.908	1.00 20.00
ATOM	2498	CA	VAL	A	090	65.821	47.903	39.051	1.00 20.00
ATOM	2499	C	VAL	A	090	64.572	48.276	39.816	1.00 20.00
ATOM	2500	O	VAL	A	090	64.276	47.684	40.843	1.00 20.00
ATOM	2501	CB	VAL	A	090	66.998	48.040	39.968	1.00 20.00
ATOM	2502	CG1	VAL	A	090	66.566	48.001	41.390	1.00 20.00
ATOM	2503	CG2	VAL	A	090	68.012	46.942	39.655	1.00 20.00
ATOM	2505	N	SER	A	091	63.807	49.232	39.295	1.00 20.00
ATOM	2506	CA	SER	A	091	62.626	49.777	39.990	1.00 20.00
ATOM	2507	C	SER	A	091	61.224	49.394	39.462	1.00 20.00

FIG. 4JJ

ATOM	2508	O	SER	A	091	60.265	49.286	40.228	1.00 20.00
ATOM	2509	CB	SER	A	091	62.780	51.317	40.030	1.00 20.00
ATOM	2510	OG	SER	A	091	63.064	51.756	41.334	1.00 20.00
ATOM	2513	N	LEU	A	092	61.125	49.264	38.146	1.00 20.00
ATOM	2514	CA	LEU	A	092	59.906	48.874	37.485	1.00 20.00
ATOM	2515	C	LEU	A	092	59.997	47.345	37.496	1.00 20.00
ATOM	2516	O	LEU	A	092	58.987	46.643	37.662	1.00 20.00
ATOM	2517	CB	LEU	A	092	59.941	49.394	36.065	1.00 20.00
ATOM	2518	CG	LEU	A	092	60.797	50.625	35.992	1.00 20.00
ATOM	2519	CD1	LEU	A	092	60.882	51.169	34.601	1.00 20.00
ATOM	2520	CD2	LEU	A	092	60.174	51.616	36.871	1.00 20.00
ATOM	2522	N	ASN	A	093	61.243	46.886	37.306	1.00 20.00
ATOM	2523	CA	ASN	A	093	61.699	45.495	37.299	1.00 20.00
ATOM	2524	C	ASN	A	093	61.214	44.889	38.582	1.00 20.00
ATOM	2525	O	ASN	A	093	60.803	43.724	38.635	1.00 20.00
ATOM	2526	CB	ASN	A	093	63.206	45.466	37.438	1.00 20.00
ATOM	2527	CG	ASN	A	093	63.927	44.920	36.244	1.00 20.00
ATOM	2528	OD1	ASN	A	093	65.126	44.666	36.350	1.00 20.00
ATOM	2529	ND2	ASN	A	093	63.245	44.739	35.117	1.00 20.00
ATOM	2533	N	ARG	A	094	61.344	45.693	39.631	1.00 20.00
ATOM	2534	CA	ARG	A	094	60.992	45.309	40.985	1.00 20.00
ATOM	2535	C	ARG	A	094	59.515	45.614	41.318	1.00 20.00
ATOM	2536	O	ARG	A	094	59.112	45.717	42.468	1.00 20.00
ATOM	2537	CB	ARG	A	094	61.954	46.010	41.937	1.00 20.00
ATOM	2538	CG	ARG	A	094	61.850	45.571	43.339	1.00 20.00
ATOM	2539	CD	ARG	A	094	62.088	46.747	44.262	1.00 20.00
ATOM	2540	NE	ARG	A	094	61.170	46.917	45.403	1.00 20.00
ATOM	2541	CZ	ARG	A	094	59.842	47.007	45.328	1.00 20.00
ATOM	2542	NH1	ARG	A	094	59.224	46.948	44.164	1.00 20.00
ATOM	2543	NH2	ARG	A	094	59.129	47.209	46.438	1.00 20.00
ATOM	2550	N	MET	A	095	58.710	45.750	40.278	1.00 20.00
ATOM	2551	CA	MET	A	095	57.306	46.018	40.421	1.00 20.00
ATOM	2552	C	MET	A	095	56.723	44.944	39.527	1.00 20.00
ATOM	2553	O	MET	A	095	55.597	44.512	39.706	1.00 20.00
ATOM	2554	CB	MET	A	095	56.967	47.406	39.870	1.00 20.00
ATOM	2555	CG	MET	A	095	57.240	48.556	40.822	1.00 20.00
ATOM	2556	SD	MET	A	095	56.618	50.279	40.365	1.00 20.00
ATOM	2557	CE	MET	A	095	56.509	50.955	42.056	1.00 20.00
ATOM	2559	N	LEU	A	096	57.495	44.509	38.551	1.00 20.00
ATOM	2560	CA	LEU	A	096	57.034	43.476	37.646	1.00 20.00
ATOM	2561	C	LEU	A	096	56.931	42.034	38.341	1.00 20.00
ATOM	2562	O	LEU	A	096	56.594	40.999	37.738	1.00 20.00
ATOM	2563	CB	LEU	A	096	57.960	43.493	36.401	1.00 20.00
ATOM	2564	CG	LEU	A	096	57.892	44.684	35.421	1.00 20.00
ATOM	2565	CD1	LEU	A	096	58.856	44.515	34.311	1.00 20.00
ATOM	2566	CD2	LEU	A	096	56.523	44.804	34.819	1.00 20.00
ATOM	2568	N	GLU	A	097	57.181	41.981	39.633	1.00 20.00
ATOM	2569	CA	GLU	A	097	57.102	40.734	40.327	1.00 20.00
ATOM	2570	C	GLU	A	097	56.396	40.934	41.642	1.00 20.00
ATOM	2571	O	GLU	A	097	57.064	41.042	42.664	1.00 20.00
ATOM	2572	CB	GLU	A	097	58.499	40.252	40.606	1.00 20.00
ATOM	2573	CG	GLU	A	097	59.459	40.519	39.475	1.00 20.00
ATOM	2574	CD	GLU	A	097	60.327	39.305	39.212	1.00 20.00
ATOM	2575	OE1	GLU	A	097	60.756	38.703	40.228	1.00 20.00
ATOM	2576	OE2	GLU	A	097	60.564	38.961	38.022	1.00 20.00
ATOM	2578	N	GLU	A	098	55.062	41.010	41.622	1.00 20.00
ATOM	2579	CA	GLU	A	098	54.192	41.177	42.823	1.00 20.00

FIG. 4KK

ATOM	2580	C	GLU	A	098	52.812	41.404	42.219	1.00	20.00
ATOM	2581	O	GLU	A	098	51.765	41.462	42.905	1.00	20.00
ATOM	2582	CB	GLU	A	098	54.514	42.433	43.686	1.00	20.00
ATOM	2583	CG	GLU	A	098	55.726	43.286	43.421	1.00	20.00
ATOM	2584	CD	GLU	A	098	56.655	43.318	44.654	1.00	20.00
ATOM	2585	OE1	GLU	A	098	56.157	43.414	45.803	1.00	20.00
ATOM	2586	OE2	GLU	A	098	57.903	43.232	44.488	1.00	20.00
ATOM	2588	N	ARG	A	099	52.872	41.529	40.898	1.00	20.00
ATOM	2589	CA	ARG	A	099	51.725	41.820	40.069	1.00	20.00
ATOM	2590	C	ARG	A	099	50.664	42.484	40.859	1.00	20.00
ATOM	2591	O	ARG	A	099	49.536	41.992	40.902	1.00	20.00
ATOM	2592	CB	ARG	A	099	51.107	40.600	39.385	1.00	20.00
ATOM	2593	CG	ARG	A	099	50.252	41.009	38.173	1.00	20.00
ATOM	2594	CD	ARG	A	099	49.462	42.327	38.402	1.00	20.00
ATOM	2595	NE	ARG	A	099	48.780	42.813	37.193	1.00	20.00
ATOM	2596	CZ	ARG	A	099	48.995	44.001	36.614	1.00	20.00
ATOM	2597	NH1	ARG	A	099	49.888	44.858	37.132	1.00	20.00
ATOM	2598	NH2	ARG	A	099	48.348	44.319	35.492	1.00	20.00
ATOM	2605	N	LYS	A	100	51.012	43.593	41.491	1.00	20.00
ATOM	2606	CA	LYS	A	100	49.996	44.273	42.208	1.00	20.00
ATOM	2607	C	LYS	A	100	49.233	45.314	41.412	1.00	20.00
ATOM	2608	O	LYS	A	100	48.414	46.009	41.961	1.00	20.00
ATOM	2609	CB	LYS	A	100	50.568	44.887	43.452	1.00	20.00
ATOM	2610	CG	LYS	A	100	49.723	44.455	44.606	1.00	20.00
ATOM	2611	CD	LYS	A	100	48.746	43.295	44.135	1.00	20.00
ATOM	2612	CE	LYS	A	100	47.476	43.250	44.951	1.00	20.00
ATOM	2613	NZ	LYS	A	100	47.799	42.986	46.386	1.00	20.00
ATOM	2618	N	THR	A	101	49.448	45.372	40.107	1.00	20.00
ATOM	2619	CA	THR	A	101	48.825	46.402	39.284	1.00	20.00
ATOM	2620	C	THR	A	101	49.208	47.748	39.873	1.00	20.00
ATOM	2621	O	THR	A	101	48.788	48.131	40.984	1.00	20.00
ATOM	2622	CB	THR	A	101	47.325	46.313	39.223	1.00	20.00
ATOM	2623	OG1	THR	A	101	46.859	45.424	40.224	1.00	20.00
ATOM	2624	CG2	THR	A	101	46.913	45.840	37.852	1.00	20.00
ATOM	2627	N	TYR	A	102	50.025	48.453	39.098	1.00	20.00
ATOM	2628	CA	TYR	A	102	50.547	49.712	39.515	1.00	20.00
ATOM	2629	C	TYR	A	102	49.870	50.826	38.785	1.00	20.00
ATOM	2630	O	TYR	A	102	49.661	51.891	39.342	1.00	20.00
ATOM	2631	CB	TYR	A	102	52.040	49.684	39.310	1.00	20.00
ATOM	2632	CG	TYR	A	102	52.744	48.940	40.406	1.00	20.00
ATOM	2633	CD1	TYR	A	102	53.416	47.744	40.169	1.00	20.00
ATOM	2634	CD2	TYR	A	102	52.769	49.460	41.663	1.00	20.00
ATOM	2635	CE1	TYR	A	102	54.090	47.122	41.160	1.00	20.00
ATOM	2636	CE2	TYR	A	102	53.430	48.852	42.653	1.00	20.00
ATOM	2637	CZ	TYR	A	102	54.102	47.691	42.416	1.00	20.00
ATOM	2638	OH	TYR	A	102	54.846	47.188	43.470	1.00	20.00
ATOM	2641	N	VAL	A	103	49.568	50.591	37.524	1.00	20.00
ATOM	2642	CA	VAL	A	103	48.790	51.544	36.741	1.00	20.00
ATOM	2643	C	VAL	A	103	47.512	50.735	36.788	1.00	20.00
ATOM	2644	O	VAL	A	103	47.571	49.547	37.137	1.00	20.00
ATOM	2645	CB	VAL	A	103	49.121	51.597	35.265	1.00	20.00
ATOM	2646	CG1	VAL	A	103	48.387	52.783	34.645	1.00	20.00
ATOM	2647	CG2	VAL	A	103	50.633	51.634	35.049	1.00	20.00
ATOM	2649	N	ASN	A	104	46.380	51.336	36.420	1.00	20.00
ATOM	2650	CA	ASN	A	104	45.109	50.645	36.473	1.00	20.00
ATOM	2651	C	ASN	A	104	44.386	51.023	35.231	1.00	20.00
ATOM	2652	O	ASN	A	104	44.569	52.110	34.731	1.00	20.00

FIG. 4LL

ATOM	2653	CB	ASN	A	104	44.360	51.089	37.714	1.00 20.00
ATOM	2654	CG	ASN	A	104	42.863	51.071	37.544	1.00 20.00
ATOM	2655	OD1	ASN	A	104	42.348	51.013	36.431	1.00 20.00
ATOM	2656	ND2	ASN	A	104	42.149	51.139	38.666	1.00 20.00
ATOM	2660	N	THR	A	105	43.545	50.137	34.732	1.00 20.00
ATOM	2661	CA	THR	A	105	42.855	50.390	33.490	1.00 20.00
ATOM	2662	C	THR	A	105	41.412	49.870	33.596	1.00 20.00
ATOM	2663	O	THR	A	105	40.678	49.783	32.593	1.00 20.00
ATOM	2664	CB	THR	A	105	43.627	49.686	32.341	1.00 20.00
ATOM	2665	OG1	THR	A	105	44.293	48.501	32.839	1.00 20.00
ATOM	2666	CG2	THR	A	105	44.686	50.595	31.792	1.00 20.00
ATOM	2669	N	THR	A	106	41.013	49.565	34.831	1.00 20.00
ATOM	2670	CA	THR	A	106	39.701	49.048	35.173	1.00 20.00
ATOM	2671	C	THR	A	106	38.588	50.103	35.353	1.00 20.00
ATOM	2672	O	THR	A	106	38.818	51.077	36.038	1.00 20.00
ATOM	2673	CB	THR	A	106	39.850	48.258	36.473	1.00 20.00
ATOM	2674	OG1	THR	A	106	39.615	46.869	36.226	1.00 20.00
ATOM	2675	CG2	THR	A	106	38.902	48.779	37.552	1.00 20.00
ATOM	2678	N	LEU	A	107	37.383	49.891	34.775	1.00 20.00
ATOM	2679	CA	LEU	A	107	36.229	50.816	34.903	1.00 20.00
ATOM	2680	C	LEU	A	107	35.437	50.546	36.199	1.00 20.00
ATOM	2681	O	LEU	A	107	35.067	49.413	36.473	1.00 20.00
ATOM	2682	CB	LEU	A	107	35.279	50.655	33.739	1.00 20.00
ATOM	2683	CG	LEU	A	107	35.798	50.744	32.313	1.00 20.00
ATOM	2684	CD1	LEU	A	107	34.625	50.728	31.345	1.00 20.00
ATOM	2685	CD2	LEU	A	107	36.667	51.987	32.120	1.00 20.00
ATOM	2687	N	TYR	A	108	35.176	51.583	36.998	1.00 20.00
ATOM	2688	CA	TYR	A	108	34.436	51.444	38.260	1.00 20.00
ATOM	2689	C	TYR	A	108	33.529	52.660	38.590	1.00 20.00
ATOM	2690	O	TYR	A	108	33.124	52.843	39.767	1.00 20.00
ATOM	2691	CB	TYR	A	108	35.417	51.219	39.419	1.00 20.00
ATOM	2692	CG	TYR	A	108	36.234	49.960	39.165	1.00 20.00
ATOM	2693	CD1	TYR	A	108	37.446	49.725	40.176	1.00 20.00
ATOM	2694	CD2	TYR	A	108	35.201	48.850	39.201	1.00 20.00
ATOM	2696	N	GLU	A	109	33.228	53.475	37.565	1.00 20.00
ATOM	2697	CA	GLU	A	109	32.363	54.664	37.691	1.00 20.00
ATOM	2698	C	GLU	A	109	33.115	55.935	37.364	1.00 20.00
ATOM	2699	O	GLU	A	109	34.039	56.360	38.093	1.00 20.00
ATOM	2700	CB	GLU	A	109	31.764	54.786	39.092	1.00 20.00
ATOM	2702	N	LYS	A	110	32.723	56.590	36.284	1.00 20.00
ATOM	2703	CA	LYS	A	110	33.431	57.801	35.968	1.00 20.00
ATOM	2704	C	LYS	A	110	34.879	57.443	35.586	1.00 20.00
ATOM	2705	O	LYS	A	110	35.653	56.902	36.366	1.00 20.00
ATOM	2706	CB	LYS	A	110	33.373	58.742	37.176	1.00 20.00
ATOM	2707	CG	LYS	A	110	32.211	58.399	38.165	1.00 20.00
ATOM	2708	CD	LYS	A	110	31.414	59.597	38.754	1.00 20.00
ATOM	2709	CE	LYS	A	110	30.154	59.092	39.514	1.00 20.00
ATOM	2710	NZ	LYS	A	110	30.320	58.678	40.967	1.00 20.00
ATOM	2715	N	PHE	A	111	35.184	57.675	34.324	1.00 20.00
ATOM	2716	CA	PHE	A	111	36.489	57.460	33.833	1.00 20.00
ATOM	2717	C	PHE	A	111	36.665	58.179	32.520	1.00 20.00
ATOM	2718	O	PHE	A	111	36.065	57.840	31.494	1.00 20.00
ATOM	2719	CB	PHE	A	111	36.842	55.994	33.658	1.00 20.00
ATOM	2720	CG	PHE	A	111	38.193	55.795	33.013	1.00 20.00
ATOM	2721	CD1	PHE	A	111	39.337	55.675	33.772	1.00 20.00
ATOM	2722	CD2	PHE	A	111	38.332	55.861	31.657	1.00 20.00
ATOM	2723	CE1	PHE	A	111	40.601	55.639	33.171	1.00 20.00

FIG. 4MM

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ATOM   2724  CE2 PHE A 111      39.575  55.824  31.077  1.00 20.00
ATOM   2725  CZ  PHE A 111      40.706  55.717  31.830  1.00 20.00
ATOM   2727  N   THR A 112      37.540  59.180  32.584  1.00 20.00
ATOM   2728  CA  THR A 112      37.904  59.997  31.457  1.00 20.00
ATOM   2729  C   THR A 112      39.374  59.703  31.350  1.00 20.00
ATOM   2730  O   THR A 112      39.967  59.297  32.329  1.00 20.00
ATOM   2731  CB  THR A 112      37.686  61.487  31.794  1.00 20.00
ATOM   2732  OG1 THR A 112      36.780  61.598  32.899  1.00 20.00
ATOM   2733  CG2 THR A 112      37.079  62.216  30.623  1.00 20.00
ATOM   2736  N   TYR A 113      39.926  59.880  30.153  1.00 20.00
ATOM   2737  CA  TYR A 113      41.339  59.706  29.866  1.00 20.00
ATOM   2738  C   TYR A 113      42.092  61.000  30.123  1.00 20.00
ATOM   2739  O   TYR A 113      41.837  61.669  31.105  1.00 20.00
ATOM   2740  CB  TYR A 113      41.520  59.320  28.433  1.00 20.00
ATOM   2741  CG  TYR A 113      41.095  57.923  28.236  1.00 20.00
ATOM   2742  CD1 TYR A 113      40.063  57.606  27.346  1.00 20.00
ATOM   2743  CD2 TYR A 113      41.699  56.879  28.960  1.00 20.00
ATOM   2744  CE1 TYR A 113      39.641  56.300  27.178  1.00 20.00
ATOM   2745  CE2 TYR A 113      41.283  55.573  28.792  1.00 20.00
ATOM   2746  CZ  TYR A 113      40.251  55.291  27.894  1.00 20.00
ATOM   2747  OH  TYR A 113      39.853  53.992  27.670  1.00 20.00
ATOM   2750  N   ALA A 114      42.958  61.423  29.201  1.00 20.00
ATOM   2751  CA  ALA A 114      43.754  62.605  29.511  1.00 20.00
ATOM   2752  C   ALA A 114      43.947  63.838  28.571  1.00 20.00
ATOM   2753  O   ALA A 114      43.604  64.944  28.952  1.00 20.00
ATOM   2754  CB  ALA A 114      45.129  62.109  30.025  1.00 20.00
ATOM   2756  N   GLY A 115      44.491  63.670  27.377  1.00 20.00
ATOM   2757  CA  GLY A 115      44.727  64.815  26.532  1.00 20.00
ATOM   2758  C   GLY A 115      44.350  64.834  25.059  1.00 20.00
ATOM   2759  O   GLY A 115      45.029  64.291  24.173  1.00 20.00
ATOM   2761  N   ILE A 116      43.220  65.504  24.838  1.00 20.00
ATOM   2762  CA  ILE A 116      42.609  65.779  23.527  1.00 20.00
ATOM   2763  C   ILE A 116      41.516  64.772  23.037  1.00 20.00
ATOM   2764  O   ILE A 116      41.123  63.952  23.880  1.00 20.00
ATOM   2765  CB  ILE A 116      43.744  65.993  22.469  1.00 20.00
ATOM   2766  OXT ILE A 116      41.049  64.815  21.867  1.00 20.00
TER
HETATM    1  C1  INH3A   1      58.776  51.045  11.645  0.00  0.00
HETATM    2  N2  INH3A   1      58.172  52.218  11.841  0.00  0.00
HETATM    3  C3  INH3A   1      58.936  53.310  12.056  0.00  0.00
HETATM    4  C4  INH3A   1      60.320  53.244  12.077  0.00  0.00
HETATM    5  C5  INH3A   1      60.887  51.924  11.859  0.00  0.00
HETATM    6  N6  INH3A   1      60.101  50.854  11.646  0.00  0.00
HETATM    8  N8  INH3A   1      58.497  54.604  12.288  0.00  0.00
HETATM    9  C9  INH3A   1      59.673  55.293  12.446  0.00  0.00
HETATM   10  C10 INH3A   1      60.842  54.525  12.326  0.00  0.00
HETATM   12  N13 INH3A   1      62.289  51.734  11.876  0.00  0.00
HETATM   13  C14 INH3A   1      62.258  54.972  12.430  0.00  0.00
HETATM   14  C16 INH3A   1      57.098  55.079  12.339  0.00  0.00
HETATM   15  C17 INH3A   1      63.049  54.530  13.477  0.00  0.00
HETATM   16  C18 INH3A   1      64.374  54.941  13.612  0.00  0.00
HETATM   17  C19 INH3A   1      64.935  55.815  12.687  0.00  0.00
HETATM   18  C20 INH3A   1      64.131  56.249  11.643  0.00  0.00
HETATM   19  C21 INH3A   1      62.810  55.841  11.508  0.00  0.00
HETATM   23  N25 INH3A   1      66.225  56.236  12.788  0.00  0.00
HETATM   24  S26 INH3A   1      66.995  56.113  14.217  0.00  0.00
HETATM   25  O27 INH3A   1      65.999  55.773  15.187  0.00  0.00
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FIG. 4NN

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HETATM   26  O28 INH3A   1      67.770  57.301  14.420  0.00  0.00
HETATM   27  C29 INH3A   1      68.100  54.741  14.032  0.00  0.00
HETATM   28  C30 INH3A   1      69.041  54.751  13.007  0.00  0.00
HETATM   29  C31 INH3A   1      69.873  53.654  12.825  0.00  0.00
HETATM   30  C32 INH3A   1      69.740  52.566  13.674  0.00  0.00
HETATM   31  C33 INH3A   1      68.801  52.539  14.696  0.00  0.00
HETATM   32  C34 INH3A   1      67.972  53.639  14.872  0.00  0.00
HETATM   37  F39 INH3A   1      70.540  51.507  13.502  0.00  0.00
HETATM   39  F41 INH3A   1      64.638  57.094  10.735  0.00  0.00
HETATM   40  C42 INH3A   1      56.781  55.784  13.669  0.00  0.00
HETATM   41  C43 INH3A   1      55.311  56.219  13.720  0.00  0.00
HETATM   42  C44 INH3A   1      54.962  57.130  12.528  0.00  0.00
HETATM   43  C45 INH3A   1      55.278  56.419  11.202  0.00  0.00
HETATM   44  C46 INH3A   1      56.748  55.981  11.144  0.00  0.00
HETATM   53  C55 INH3A   1      53.385  58.715  13.548  0.00  0.00
HETATM   54  C56 INH3A   1      51.998  59.356  13.419  0.00  0.00
HETATM   55  N57 INH3A   1      50.930  58.353  13.520  0.00  0.00
HETATM   56  C58 INH3A   1      51.136  57.302  12.516  0.00  0.00
HETATM   57  C59 INH3A   1      52.522  56.662  12.658  0.00  0.00
HETATM   58  N60 INH3A   1      53.588  57.668  12.536  0.00  0.00
HETATM   68  C70 INH3A   1      49.599  58.958  13.416  0.00  0.00
TER
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FIG. 4OO

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CRYST    86.000   86.000  112.000  90.00  90.00  90.00 P42212
SCALE1      0.01163  0.00000  0.00000        0.00000
SCALE2      0.00000  0.01163  0.00000        0.00000
SCALE3      0.00000  0.00000  0.00893        0.00000
ATOM      1  N   PRO A 817       8.606  38.803   6.968  1.00 63.06
ATOM      2  CA  PRO A 817       9.750  39.629   6.436  1.00 62.53
ATOM      3  C   PRO A 817      10.180  38.953   5.133  1.00 62.97
ATOM      4  O   PRO A 817      10.749  37.851   5.149  1.00 59.85
ATOM      5  CB  PRO A 817      10.807  39.752   7.499  1.00 62.45
ATOM      6  N   VAL A 818       9.794  39.542   3.998  1.00 63.22
ATOM      7  CA  VAL A 818      10.112  38.916   2.711  1.00 66.18
ATOM      8  C   VAL A 818      11.172  39.708   1.952  1.00 67.24
ATOM      9  O   VAL A 818      11.086  40.927   1.837  1.00 68.73
ATOM     10  CB  VAL A 818       8.866  38.691   1.843  1.00 66.96
ATOM     11  CG1 VAL A 818       9.133  37.632   0.770  1.00 67.29
ATOM     12  CG2 VAL A 818       7.637  38.224   2.629  1.00 66.80
ATOM     13  N   LEU A 819      12.192  39.014   1.464  1.00 67.40
ATOM     14  CA  LEU A 819      13.300  39.569   0.705  1.00 67.89
ATOM     15  C   LEU A 819      13.445  38.938  -0.680  1.00 68.53
ATOM     16  O   LEU A 819      13.179  37.750  -0.875  1.00 67.98
ATOM     17  CB  LEU A 819      14.589  39.374   1.493  1.00 67.17
ATOM     18  N   ASP A 820      13.854  39.728  -1.668  1.00 70.32
ATOM     19  CA  ASP A 820      13.962  39.181  -3.018  1.00 74.15
ATOM     20  C   ASP A 820      15.382  38.826  -3.421  1.00 75.07
ATOM     21  O   ASP A 820      16.390  39.377  -2.978  1.00 74.87
ATOM     22  CB  ASP A 820      13.314  40.147  -4.017  1.00 76.15
ATOM     23  CG  ASP A 820      13.968  41.518  -4.054  1.00 78.23
ATOM     24  OD1 ASP A 820      14.712  41.846  -3.092  1.00 79.04
ATOM     25  OD2 ASP A 820      13.712  42.246  -5.051  1.00 78.55
ATOM     26  N   TRP A 821      15.489  37.870  -4.336  1.00 77.12
ATOM     27  CA  TRP A 821      16.794  37.480  -4.871  1.00 80.00
ATOM     28  C   TRP A 821      17.288  38.671  -5.674  1.00 80.90
ATOM     29  O   TRP A 821      16.560  39.677  -5.750  1.00 82.56
ATOM     30  CB  TRP A 821      16.640  36.237  -5.738  1.00 81.50
ATOM     31  CG  TRP A 821      17.979  35.683  -6.126  1.00 84.29
ATOM     32  CD1 TRP A 821      18.770  36.052  -7.174  1.00 85.04
ATOM     33  CD2 TRP A 821      18.686  34.639  -5.443  1.00 85.54
ATOM     34  NE1 TRP A 821      19.932  35.323  -7.184  1.00 85.91
ATOM     35  CE2 TRP A 821      19.895  34.435  -6.138  1.00 86.16
ATOM     36  CE3 TRP A 821      18.402  33.854  -4.317  1.00 85.72
ATOM     37  CZ2 TRP A 821      20.822  33.474  -5.736  1.00 86.76
ATOM     38  CZ3 TRP A 821      19.317  32.899  -3.914  1.00 86.12
ATOM     39  CH2 TRP A 821      20.513  32.723  -4.632  1.00 86.81
ATOM     40  N   ASN A 822      18.490  38.703  -6.220  1.00 80.99
ATOM     41  CA  ASN A 822      18.941  39.868  -6.995  1.00 81.52
ATOM     42  C   ASN A 822      18.729  41.071  -6.079  1.00 80.56
ATOM     43  O   ASN A 822      18.110  42.084  -6.381  1.00 81.67
ATOM     44  CB  ASN A 822      18.164  39.937  -8.312  1.00 83.00
ATOM     45  CG  ASN A 822      19.059  40.084  -9.532  1.00 84.08
ATOM     46  OD1 ASN A 822      20.168  40.617  -9.420  1.00 84.25
ATOM     47  ND2 ASN A 822      18.581  39.608 -10.679  1.00 84.49
ATOM     48  N   ASP A 823      19.204  40.923  -4.856  1.00 78.69
ATOM     49  CA  ASP A 823      19.120  41.815  -3.723  1.00 76.89
ATOM     50  C   ASP A 823      19.874  41.123  -2.568  1.00 74.92
ATOM     51  O   ASP A 823      19.952  41.542  -1.417  1.00 75.11
ATOM     52  CB  ASP A 823      17.695  42.112  -3.299  1.00 77.66
ATOM     53  CG  ASP A 823      17.306  43.572  -3.217  1.00 78.83
```

FIG. 5A

ATOM	54	OD1	ASP	A	823	17.885	44.406	-3.955	1.00	79.53
ATOM	55	OD2	ASP	A	823	16.391	43.945	-2.444	1.00	78.52
ATOM	56	N	ILE	A	824	20.438	39.973	-2.919	1.00	71.67
ATOM	57	CA	ILE	A	824	21.270	39.189	-2.030	1.00	69.30
ATOM	58	C	ILE	A	824	22.624	39.046	-2.750	1.00	67.35
ATOM	59	O	ILE	A	824	22.678	38.352	-3.770	1.00	65.47
ATOM	60	CB	ILE	A	824	20.744	37.783	-1.696	1.00	69.43
ATOM	61	CG1	ILE	A	824	19.356	37.733	-1.074	1.00	69.93
ATOM	62	CG2	ILE	A	824	21.752	37.046	-0.820	1.00	69.07
ATOM	63	CD1	ILE	A	824	19.156	38.009	0.386	1.00	71.48
ATOM	64	N	LYS	A	825	23.649	39.735	-2.252	1.00	65.03
ATOM	65	CA	LYS	A	825	24.977	39.581	-2.829	1.00	63.66
ATOM	66	C	LYS	A	825	25.810	38.677	-1.903	1.00	62.88
ATOM	67	O	LYS	A	825	26.290	39.103	-0.850	1.00	60.46
ATOM	68	CB	LYS	A	825	25.688	40.893	-3.082	1.00	63.33
ATOM	69	N	PHE	A	826	25.952	37.420	-2.315	1.00	62.22
ATOM	70	CA	PHE	A	826	26.745	36.434	-1.595	1.00	63.65
ATOM	71	C	PHE	A	826	28.243	36.752	-1.654	1.00	64.85
ATOM	72	O	PHE	A	826	28.806	36.978	-2.738	1.00	65.98
ATOM	73	CB	PHE	A	826	26.535	35.019	-2.151	1.00	63.23
ATOM	74	CG	PHE	A	826	25.242	34.324	-1.828	1.00	63.28
ATOM	75	CD1	PHE	A	826	24.194	34.262	-2.742	1.00	63.47
ATOM	76	CD2	PHE	A	826	25.068	33.738	-0.587	1.00	62.78
ATOM	77	CE1	PHE	A	826	23.013	33.606	-2.421	1.00	63.26
ATOM	78	CE2	PHE	A	826	23.893	33.090	-0.261	1.00	63.76
ATOM	79	CZ	PHE	A	826	22.859	33.026	-1.183	1.00	63.42
ATOM	80	N	GLN	A	827	28.933	36.771	-0.514	1.00	64.73
ATOM	81	CA	GLN	A	827	30.359	37.048	-0.474	1.00	63.67
ATOM	82	C	GLN	A	827	31.182	35.763	-0.387	1.00	62.27
ATOM	83	O	GLN	A	827	31.703	35.217	-1.356	1.00	61.84
ATOM	84	CB	GLN	A	827	30.736	37.884	0.748	1.00	65.45
ATOM	85	CG	GLN	A	827	29.641	38.676	1.428	1.00	69.14
ATOM	86	CD	GLN	A	827	29.805	40.166	1.185	1.00	71.09
ATOM	87	OE1	GLN	A	827	29.364	40.617	0.124	1.00	72.36
ATOM	88	NE2	GLN	A	827	30.442	40.865	2.124	1.00	71.89
ATOM	89	N	ASP	A	828	31.371	35.286	0.838	1.00	61.57
ATOM	90	CA	ASP	A	828	32.237	34.122	1.034	1.00	62.37
ATOM	91	C	ASP	A	828	31.576	33.071	1.883	1.00	61.37
ATOM	92	O	ASP	A	828	30.330	32.899	1.910	1.00	63.34
ATOM	93	CB	ASP	A	828	33.605	34.623	1.532	1.00	63.30
ATOM	94	CG	ASP	A	828	33.536	35.073	2.977	1.00	65.22
ATOM	95	OD1	ASP	A	828	34.629	35.346	3.505	1.00	66.32
ATOM	96	OD2	ASP	A	828	32.418	35.135	3.513	1.00	67.27
ATOM	97	N	VAL	A	829	32.332	32.174	2.503	1.00	59.16
ATOM	98	CA	VAL	A	829	31.820	31.095	3.339	1.00	56.81
ATOM	99	C	VAL	A	829	32.101	31.413	4.805	1.00	57.13
ATOM	100	O	VAL	A	829	33.252	31.767	5.119	1.00	57.41
ATOM	101	CB	VAL	A	829	32.462	29.753	2.948	1.00	55.58
ATOM	102	CG1	VAL	A	829	32.035	28.658	3.909	1.00	55.56
ATOM	103	CG2	VAL	A	829	32.111	29.383	1.513	1.00	55.17
ATOM	104	N	ILE	A	830	31.106	31.314	5.693	1.00	56.36
ATOM	105	CA	ILE	A	830	31.360	31.613	7.108	1.00	54.69
ATOM	106	C	ILE	A	830	31.971	30.371	7.750	1.00	54.51
ATOM	107	O	ILE	A	830	32.927	30.411	8.507	1.00	54.88
ATOM	108	CB	ILE	A	830	30.170	32.157	7.898	1.00	52.84
ATOM	109	CG1	ILE	A	830	29.780	33.560	7.374	1.00	52.48
ATOM	110	CG2	ILE	A	830	30.518	32.300	9.375	1.00	51.14

FIG. 5B

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ATOM    111  CD1 ILE A 830      28.389  34.012   7.808  1.00 52.01
ATOM    112  N   GLY A 831      31.431  29.232   7.376  1.00 54.93
ATOM    113  CA  GLY A 831      31.949  27.959   7.866  1.00 57.73
ATOM    114  C   GLY A 831      30.703  27.066   7.878  1.00 60.30
ATOM    115  O   GLY A 831      29.687  27.433   7.281  1.00 59.66
ATOM    116  N   GLU A 832      30.811  25.963   8.594  1.00 62.36
ATOM    117  CA  GLU A 832      29.649  25.080   8.634  1.00 65.54
ATOM    118  C   GLU A 832      28.918  25.256   9.956  1.00 67.03
ATOM    119  O   GLU A 832      29.525  25.480  10.982  1.00 65.58
ATOM    120  CB  GLU A 832      30.079  23.647   8.389  1.00 65.24
ATOM    121  CG  GLU A 832      29.979  22.748   9.615  1.00 64.68
ATOM    122  CD  GLU A 832      30.771  21.493   9.247  1.00 65.38
ATOM    123  OE1 GLU A 832      31.871  21.394   9.838  1.00 65.15
ATOM    124  OE2 GLU A 832      30.232  20.771   8.386  1.00 64.01
ATOM    125  N   GLY A 833      27.605  25.128   9.870  1.00 71.16
ATOM    126  CA  GLY A 833      26.741  25.268  11.048  1.00 75.85
ATOM    127  C   GLY A 833      25.973  23.945  11.138  1.00 79.10
ATOM    128  O   GLY A 833      26.489  22.959  11.666  1.00 80.05
ATOM    129  N   ASN A 834      24.750  23.982  10.627  1.00 80.77
ATOM    130  CA  ASN A 834      23.887  22.807  10.614  1.00 82.57
ATOM    131  C   ASN A 834      23.055  22.917   9.332  1.00 82.72
ATOM    132  O   ASN A 834      22.709  24.047   8.973  1.00 83.47
ATOM    133  CB  ASN A 834      22.974  22.712  11.826  1.00 83.64
ATOM    134  CG  ASN A 834      23.565  22.227  13.122  1.00 84.87
ATOM    135  OD1 ASN A 834      23.040  22.476  14.214  1.00 85.57
ATOM    136  ND2 ASN A 834      24.692  21.516  13.114  1.00 85.28
ATOM    137  N   PHE A 835      22.813  21.799   8.663  1.00 82.37
ATOM    138  CA  PHE A 835      22.018  21.747   7.436  1.00 81.44
ATOM    139  C   PHE A 835      22.770  22.311   6.227  1.00 79.71
ATOM    140  O   PHE A 835      22.207  22.742   5.221  1.00 80.02
ATOM    141  CB  PHE A 835      20.656  22.423   7.609  1.00 81.62
ATOM    142  N   GLY A 836      24.093  22.257   6.306  1.00 77.25
ATOM    143  CA  GLY A 836      25.011  22.771   5.308  1.00 73.64
ATOM    144  C   GLY A 836      25.714  24.008   5.875  1.00 70.61
ATOM    145  O   GLY A 836      25.485  24.453   7.008  1.00 71.32
ATOM    146  N   GLN A 837      26.589  24.607   5.081  1.00 67.00
ATOM    147  CA  GLN A 837      27.288  25.779   5.584  1.00 64.94
ATOM    148  C   GLN A 837      26.303  26.943   5.749  1.00 61.14
ATOM    149  O   GLN A 837      25.079  26.947   5.627  1.00 62.09
ATOM    150  CB  GLN A 837      28.510  26.214   4.782  1.00 65.56
ATOM    151  CG  GLN A 837      28.323  26.175   3.277  1.00 68.22
ATOM    152  CD  GLN A 837      28.499  24.771   2.717  1.00 70.10
ATOM    153  OE1 GLN A 837      27.540  23.989   2.498  1.00 71.35
ATOM    154  NE2 GLN A 837      29.776  24.447   2.508  1.00 69.74
ATOM    155  N   VAL A 838      26.949  27.991   6.223  1.00 56.19
ATOM    156  CA  VAL A 838      26.368  29.284   6.530  1.00 52.12
ATOM    157  C   VAL A 838      27.166  30.196   5.612  1.00 51.49
ATOM    158  O   VAL A 838      28.401  30.088   5.669  1.00 50.02
ATOM    159  CB  VAL A 838      26.657  29.586   8.002  1.00 50.54
ATOM    160  CG1 VAL A 838      26.258  30.989   8.386  1.00 48.67
ATOM    161  CG2 VAL A 838      25.974  28.553   8.890  1.00 48.75
ATOM    162  N   LEU A 839      26.512  30.915   4.719  1.00 50.28
ATOM    163  CA  LEU A 839      27.308  31.782   3.831  1.00 48.12
ATOM    164  C   LEU A 839      27.210  33.217   4.324  1.00 48.21
ATOM    165  O   LEU A 839      26.364  33.580   5.139  1.00 46.74
ATOM    166  CB  LEU A 839      26.831  31.625   2.395  1.00 47.75
ATOM    167  CG  LEU A 839      26.828  30.229   1.803  1.00 48.45
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FIG. 5C

ATOM	168	CD1	LEU	A	839	26.155	30.260	0.433	1.00	47.96
ATOM	169	CD2	LEU	A	839	28.160	29.519	1.717	1.00	44.56
ATOM	170	N	LYS	A	840	28.053	34.107	3.847	1.00	47.52
ATOM	171	CA	LYS	A	840	27.984	35.508	4.234	1.00	48.47
ATOM	172	C	LYS	A	840	27.434	36.369	3.109	1.00	49.26
ATOM	173	O	LYS	A	840	27.837	36.150	1.960	1.00	49.21
ATOM	174	CB	LYS	A	840	29.393	35.943	4.654	1.00	48.66
ATOM	175	CG	LYS	A	840	29.320	37.059	5.668	1.00	49.85
ATOM	176	CD	LYS	A	840	29.716	38.398	5.125	1.00	49.60
ATOM	177	CE	LYS	A	840	29.768	39.457	6.225	1.00	50.13
ATOM	178	NZ	LYS	A	840	31.184	39.749	6.580	1.00	51.35
ATOM	179	N	ALA	A	841	26.486	37.270	3.389	1.00	51.52
ATOM	180	CA	ALA	A	841	25.968	38.108	2.312	1.00	53.29
ATOM	181	C	ALA	A	841	25.768	39.564	2.726	1.00	54.51
ATOM	182	O	ALA	A	841	25.753	39.914	3.903	1.00	54.20
ATOM	183	CB	ALA	A	841	24.641	37.503	1.837	1.00	52.47
ATOM	184	N	ARG	A	842	25.564	40.398	1.714	1.00	57.16
ATOM	185	CA	ARG	A	842	25.154	41.784	1.915	1.00	60.23
ATOM	186	C	ARG	A	842	23.699	41.667	1.451	1.00	61.88
ATOM	187	O	ARG	A	842	23.499	41.023	0.416	1.00	63.40
ATOM	188	CB	ARG	A	842	25.900	42.835	1.119	1.00	61.09
ATOM	189	CG	ARG	A	842	27.301	43.137	1.622	1.00	62.77
ATOM	190	CD	ARG	A	842	27.258	43.791	2.995	1.00	63.72
ATOM	191	NE	ARG	A	842	26.985	45.231	2.928	1.00	64.65
ATOM	192	CZ	ARG	A	842	26.963	45.986	4.017	1.00	65.52
ATOM	193	NH1	ARG	A	842	26.724	47.291	4.022	1.00	65.78
ATOM	194	NH2	ARG	A	842	27.158	45.436	5.214	1.00	66.80
ATOM	195	N	ILE	A	843	22.745	42.047	2.281	1.00	63.86
ATOM	196	CA	ILE	A	843	21.322	41.935	1.983	1.00	66.38
ATOM	197	C	ILE	A	843	20.610	43.284	2.150	1.00	69.29
ATOM	198	O	ILE	A	843	20.337	43.810	3.233	1.00	72.01
ATOM	199	CB	ILE	A	843	20.524	40.846	2.715	1.00	64.76
ATOM	200	CG1	ILE	A	843	20.218	41.134	4.182	1.00	63.75
ATOM	201	CG2	ILE	A	843	21.198	39.477	2.638	1.00	65.06
ATOM	202	CD1	ILE	A	843	19.030	40.372	4.733	1.00	61.60
ATOM	203	N	LYS	A	844	20.274	43.844	0.975	1.00	70.72
ATOM	204	CA	LYS	A	844	19.599	45.144	0.939	1.00	72.14
ATOM	205	C	LYS	A	844	18.157	45.087	1.427	1.00	73.85
ATOM	206	O	LYS	A	844	17.234	44.834	0.650	1.00	74.26
ATOM	207	CB	LYS	A	844	19.596	45.771	-0.449	1.00	71.35
ATOM	208	N	LYS	A	845	17.931	45.392	2.697	1.00	75.42
ATOM	209	CA	LYS	A	845	16.580	45.403	3.262	1.00	77.81
ATOM	210	C	LYS	A	845	16.190	46.868	3.403	1.00	80.30
ATOM	211	O	LYS	A	845	16.751	47.630	4.197	1.00	79.71
ATOM	212	CB	LYS	A	845	16.528	44.624	4.561	1.00	77.32
ATOM	213	CG	LYS	A	845	15.188	44.450	5.231	1.00	76.89
ATOM	214	CD	LYS	A	845	15.318	43.734	6.572	1.00	76.27
ATOM	215	CE	LYS	A	845	13.956	43.469	7.205	1.00	75.52
ATOM	216	NZ	LYS	A	845	14.066	42.788	8.521	1.00	74.44
ATOM	217	N	ASP	A	846	15.243	47.333	2.610	1.00	82.92
ATOM	218	CA	ASP	A	846	14.674	48.627	2.374	1.00	84.85
ATOM	219	C	ASP	A	846	15.649	49.493	1.560	1.00	85.22
ATOM	220	O	ASP	A	846	15.804	49.302	0.353	1.00	85.44
ATOM	221	CB	ASP	A	846	14.070	49.395	3.514	1.00	86.44
ATOM	222	CG	ASP	A	846	14.770	49.744	4.790	1.00	87.92
ATOM	223	OD1	ASP	A	846	15.058	50.942	5.029	1.00	88.52
ATOM	224	OD2	ASP	A	846	15.044	48.819	5.599	1.00	89.21

FIG. 5D

ATOM	225	N	GLY	A	847	16.337	50.395	2.231	1.00 85.08
ATOM	226	CA	GLY	A	847	17.317	51.266	1.590	1.00 83.96
ATOM	227	C	GLY	A	847	18.593	51.154	2.430	1.00 83.43
ATOM	228	O	GLY	A	847	19.555	51.871	2.210	1.00 84.91
ATOM	229	N	LEU	A	848	18.493	50.239	3.396	1.00 81.24
ATOM	230	CA	LEU	A	848	19.634	49.951	4.250	1.00 78.49
ATOM	231	C	LEU	A	848	20.311	48.732	3.617	1.00 76.61
ATOM	232	O	LEU	A	848	19.608	47.760	3.340	1.00 76.98
ATOM	233	CB	LEU	A	848	19.195	49.564	5.658	1.00 78.88
ATOM	234	CG	LEU	A	848	18.312	50.582	6.388	1.00 79.08
ATOM	235	CD1	LEU	A	848	17.346	49.858	7.312	1.00 79.29
ATOM	236	CD2	LEU	A	848	19.184	51.563	7.157	1.00 79.32
ATOM	237	N	ARG	A	849	21.592	48.863	3.326	1.00 73.72
ATOM	238	CA	ARG	A	849	22.332	47.696	2.850	1.00 70.15
ATOM	239	C	ARG	A	849	22.830	47.095	4.175	1.00 67.06
ATOM	240	O	ARG	A	849	23.153	47.922	5.036	1.00 65.85
ATOM	241	CB	ARG	A	849	23.493	48.031	1.941	1.00 71.56
ATOM	242	CG	ARG	A	849	23.308	47.798	0.452	1.00 72.96
ATOM	243	CD	ARG	A	849	24.483	46.995	-0.110	1.00 74.22
ATOM	244	NE	ARG	A	849	25.606	47.792	-0.586	1.00 75.64
ATOM	245	CZ	ARG	A	849	26.848	47.399	-0.871	1.00 75.22
ATOM	246	NH1	ARG	A	849	27.183	46.121	-0.715	1.00 73.54
ATOM	247	NH2	ARG	A	849	27.739	48.290	-1.305	1.00 74.94
ATOM	248	N	MET	A	850	22.777	45.781	4.369	1.00 63.25
ATOM	249	CA	MET	A	850	23.293	45.285	5.655	1.00 59.28
ATOM	250	C	MET	A	850	23.898	43.883	5.493	1.00 55.95
ATOM	251	O	MET	A	850	23.690	43.197	4.494	1.00 56.07
ATOM	252	CB	MET	A	850	22.245	45.279	6.757	1.00 58.62
ATOM	253	CG	MET	A	850	21.296	44.096	6.631	1.00 59.21
ATOM	254	SD	MET	A	850	19.724	44.280	7.443	1.00 59.73
ATOM	255	CE	MET	A	850	20.128	44.922	9.049	1.00 59.43
ATOM	256	N	ASP	A	851	24.651	43.563	6.548	1.00 51.79
ATOM	257	CA	ASP	A	851	25.299	42.268	6.600	1.00 48.61
ATOM	258	C	ASP	A	851	24.332	41.192	7.084	1.00 45.57
ATOM	259	O	ASP	A	851	23.630	41.457	8.086	1.00 42.14
ATOM	260	CB	ASP	A	851	26.379	42.285	7.697	1.00 50.01
ATOM	261	CG	ASP	A	851	27.669	42.933	7.256	1.00 50.84
ATOM	262	OD1	ASP	A	851	28.043	42.801	6.057	1.00 51.87
ATOM	263	OD2	ASP	A	851	28.272	43.563	8.144	1.00 50.81
ATOM	264	N	ALA	A	852	24.472	39.961	6.632	1.00 45.45
ATOM	265	CA	ALA	A	852	23.622	38.884	7.138	1.00 42.89
ATOM	266	C	ALA	A	852	24.373	37.570	7.066	1.00 42.71
ATOM	267	O	ALA	A	852	25.336	37.518	6.303	1.00 43.78
ATOM	268	CB	ALA	A	852	22.397	38.727	6.261	1.00 41.61
ATOM	269	N	ALA	A	853	23.847	36.577	7.785	1.00 43.18
ATOM	270	CA	ALA	A	853	24.394	35.222	7.668	1.00 43.19
ATOM	271	C	ALA	A	853	23.300	34.446	6.931	1.00 45.23
ATOM	272	O	ALA	A	853	22.122	34.570	7.296	1.00 45.40
ATOM	273	CB	ALA	A	853	24.725	34.651	9.043	1.00 43.45
ATOM	274	N	ILE	A	854	23.599	33.717	5.863	1.00 45.69
ATOM	275	CA	ILE	A	854	22.561	33.051	5.093	1.00 46.79
ATOM	276	C	ILE	A	854	22.583	31.537	5.228	1.00 50.11
ATOM	277	O	ILE	A	854	23.643	30.913	5.101	1.00 51.97
ATOM	278	CB	ILE	A	854	22.686	33.334	3.581	1.00 45.28
ATOM	279	CG1	ILE	A	854	22.754	34.819	3.268	1.00 45.20
ATOM	280	CG2	ILE	A	854	21.553	32.685	2.794	1.00 45.13
ATOM	281	CD1	ILE	A	854	21.509	35.654	3.433	1.00 45.48

FIG. 5E

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ATOM    282  N   LYS A 855      21.408  30.949   5.453  1.00 51.72
ATOM    283  CA  LYS A 855      21.355  29.474   5.425  1.00 54.33
ATOM    284  C   LYS A 855      20.240  29.052   4.458  1.00 55.89
ATOM    285  O   LYS A 855      19.276  29.786   4.205  1.00 52.41
ATOM    286  CB  LYS A 855      21.271  28.892   6.808  1.00 55.64
ATOM    287  CG  LYS A 855      19.914  28.834   7.487  1.00 58.25
ATOM    288  CD  LYS A 855      20.052  28.092   8.807  1.00 59.55
ATOM    289  CE  LYS A 855      18.987  27.027   9.025  1.00 60.12
ATOM    290  NZ  LYS A 855      19.484  26.165  10.151  1.00 60.89
ATOM    291  N   ARG A 856      20.386  27.871   3.871  1.00 59.82
ATOM    292  CA  ARG A 856      19.419  27.341   2.915  1.00 63.71
ATOM    293  C   ARG A 856      18.809  26.009   3.309  1.00 66.24
ATOM    294  O   ARG A 856      19.456  25.004   3.565  1.00 66.29
ATOM    295  CB  ARG A 856      20.126  27.258   1.555  1.00 63.38
ATOM    296  N   MET A 857      17.486  25.951   3.418  1.00 69.77
ATOM    297  CA  MET A 857      16.718  24.748   3.728  1.00 73.04
ATOM    298  C   MET A 857      15.960  24.381   2.447  1.00 75.83
ATOM    299  O   MET A 857      16.149  25.126   1.472  1.00 77.44
ATOM    300  CB  MET A 857      15.761  24.965   4.887  1.00 72.49
ATOM    301  N   LYS A 858      15.174  23.321   2.404  1.00 78.15
ATOM    302  CA  LYS A 858      14.449  22.985   1.184  1.00 80.35
ATOM    303  C   LYS A 858      13.181  22.168   1.417  1.00 81.76
ATOM    304  O   LYS A 858      13.118  21.298   2.282  1.00 82.29
ATOM    305  CB  LYS A 858      15.320  22.196   0.212  1.00 80.34
ATOM    306  N   GLU A 859      12.171  22.427   0.593  1.00 82.86
ATOM    307  CA  GLU A 859      10.905  21.705   0.631  1.00 83.98
ATOM    308  C   GLU A 859      10.372  21.378   2.024  1.00 84.84
ATOM    309  O   GLU A 859       9.465  20.540   2.160  1.00 85.54
ATOM    310  CB  GLU A 859      11.040  20.388  -0.143  1.00 83.34
TER
ATOM    311  N   ASP B 868       3.887  24.257   9.102  1.00 74.33
ATOM    312  CA  ASP B 868       4.969  23.506   9.742  1.00 73.45
ATOM    313  C   ASP B 868       6.151  24.465   9.894  1.00 72.92
ATOM    314  O   ASP B 868       6.215  25.236  10.848  1.00 72.75
ATOM    315  CB  ASP B 868       5.345  22.276   8.927  1.00 73.09
ATOM    316  N   PHE B 869       6.973  24.491   8.845  1.00 71.93
ATOM    317  CA  PHE B 869       8.128  25.356   8.739  1.00 71.39
ATOM    318  C   PHE B 869       7.722  26.812   8.514  1.00 69.85
ATOM    319  O   PHE B 869       8.507  27.721   8.789  1.00 68.53
ATOM    320  CB  PHE B 869       9.086  24.894   7.635  1.00 72.16
ATOM    321  N   ALA B 870       6.485  27.041   8.084  1.00 68.66
ATOM    322  CA  ALA B 870       6.008  28.412   7.917  1.00 67.79
ATOM    323  C   ALA B 870       5.699  28.972   9.300  1.00 66.69
ATOM    324  O   ALA B 870       5.914  30.142   9.612  1.00 67.76
ATOM    325  CB  ALA B 870       4.786  28.421   7.009  1.00 67.73
ATOM    326  N   GLY B 871       5.125  28.124  10.156  1.00 64.74
ATOM    327  CA  GLY B 871       4.746  28.539  11.506  1.00 63.48
ATOM    328  C   GLY B 871       5.968  28.696  12.407  1.00 63.38
ATOM    329  O   GLY B 871       6.078  29.586  13.241  1.00 62.27
ATOM    330  N   GLU B 872       6.936  27.789  12.259  1.00 63.08
ATOM    331  CA  GLU B 872       8.163  27.830  13.033  1.00 62.41
ATOM    332  C   GLU B 872       8.870  29.166  12.865  1.00 59.48
ATOM    333  O   GLU B 872       9.299  29.759  13.849  1.00 59.18
ATOM    334  CB  GLU B 872       9.104  26.684  12.627  1.00 64.92
ATOM    335  CG  GLU B 872       8.756  25.334  13.218  1.00 67.28
ATOM    336  CD  GLU B 872       9.191  24.093  12.474  1.00 68.33
ATOM    337  OE1 GLU B 872       8.848  22.953  12.910  1.00 69.51
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FIG. 5F

ATOM	338	OE2	GLU	B	872	9.882	24.117	11.435	1.00	69.53
ATOM	339	N	LEU	B	873	9.004	29.664	11.648	1.00	57.71
ATOM	340	CA	LEU	B	873	9.635	30.916	11.312	1.00	55.15
ATOM	341	C	LEU	B	873	8.988	32.099	12.034	1.00	55.46
ATOM	342	O	LEU	B	873	9.656	33.045	12.483	1.00	53.19
ATOM	343	CB	LEU	B	873	9.629	31.206	9.816	1.00	54.80
ATOM	344	CG	LEU	B	873	10.436	30.326	8.876	1.00	56.52
ATOM	345	CD1	LEU	B	873	10.416	30.920	7.466	1.00	56.98
ATOM	346	CD2	LEU	B	873	11.886	30.139	9.305	1.00	57.06
ATOM	347	N	GLU	B	874	7.663	32.055	12.083	1.00	53.38
ATOM	348	CA	GLU	B	874	6.839	33.058	12.743	1.00	53.73
ATOM	349	C	GLU	B	874	7.208	33.198	14.215	1.00	50.89
ATOM	350	O	GLU	B	874	7.431	34.279	14.773	1.00	48.19
ATOM	351	CB	GLU	B	874	5.379	32.579	12.639	1.00	57.54
ATOM	352	CG	GLU	B	874	4.388	33.300	13.533	1.00	61.33
ATOM	353	CD	GLU	B	874	3.007	32.638	13.433	1.00	64.62
ATOM	354	OE1	GLU	B	874	2.075	33.216	14.045	1.00	66.21
ATOM	355	OE2	GLU	B	874	2.876	31.577	12.771	1.00	64.60
ATOM	356	N	VAL	B	875	7.278	32.004	14.839	1.00	48.16
ATOM	357	CA	VAL	B	875	7.665	31.965	16.266	1.00	47.64
ATOM	358	C	VAL	B	875	9.051	32.599	16.426	1.00	46.85
ATOM	359	O	VAL	B	875	9.211	33.498	17.257	1.00	45.14
ATOM	360	CB	VAL	B	875	7.523	30.545	16.799	1.00	47.78
ATOM	361	CG1	VAL	B	875	8.477	30.264	17.946	1.00	48.21
ATOM	362	CG2	VAL	B	875	6.077	30.272	17.240	1.00	47.41
ATOM	363	N	LEU	B	876	10.000	32.278	15.538	1.00	47.87
ATOM	364	CA	LEU	B	876	11.348	32.838	15.552	1.00	50.02
ATOM	365	C	LEU	B	876	11.435	34.322	15.245	1.00	50.20
ATOM	366	O	LEU	B	876	12.285	34.988	15.845	1.00	51.04
ATOM	367	CB	LEU	B	876	12.308	32.074	14.611	1.00	48.16
ATOM	368	CG	LEU	B	876	12.598	30.663	15.159	1.00	49.64
ATOM	369	CD1	LEU	B	876	13.303	29.816	14.116	1.00	48.69
ATOM	370	CD2	LEU	B	876	13.407	30.766	16.452	1.00	51.42
ATOM	371	N	CYS	B	877	10.607	34.849	14.358	1.00	50.72
ATOM	372	CA	CYS	B	877	10.638	36.276	14.029	1.00	51.41
ATOM	373	C	CYS	B	877	10.130	37.090	15.215	1.00	50.29
ATOM	374	O	CYS	B	877	10.630	38.171	15.550	1.00	49.69
ATOM	375	CB	CYS	B	877	9.777	36.555	12.788	1.00	53.49
ATOM	376	SG	CYS	B	877	9.320	38.304	12.668	1.00	56.75
ATOM	377	N	LYS	B	878	9.155	36.480	15.922	1.00	49.77
ATOM	378	CA	LYS	B	878	8.602	37.082	17.122	1.00	49.11
ATOM	379	C	LYS	B	878	9.567	37.033	18.298	1.00	47.30
ATOM	380	O	LYS	B	878	9.418	37.925	19.128	1.00	47.68
ATOM	381	CB	LYS	B	878	7.284	36.415	17.561	1.00	51.27
ATOM	382	CG	LYS	B	878	6.097	36.821	16.728	1.00	53.14
ATOM	383	CD	LYS	B	878	5.072	35.740	16.473	1.00	55.56
ATOM	384	CE	LYS	B	878	4.132	35.453	17.638	1.00	55.88
ATOM	385	NZ	LYS	B	878	3.445	34.138	17.433	1.00	57.41
ATOM	386	N	LEU	B	879	10.495	36.091	18.403	1.00	44.23
ATOM	387	CA	LEU	B	879	11.388	36.049	19.550	1.00	42.64
ATOM	388	C	LEU	B	879	12.665	36.881	19.317	1.00	41.06
ATOM	389	O	LEU	B	879	13.291	37.300	20.264	1.00	39.35
ATOM	390	CB	LEU	B	879	11.857	34.606	19.819	1.00	41.39
ATOM	391	CG	LEU	B	879	10.790	33.580	20.246	1.00	40.34
ATOM	392	CD1	LEU	B	879	11.327	32.180	20.076	1.00	40.43
ATOM	393	CD2	LEU	B	879	10.378	33.826	21.693	1.00	40.68
ATOM	394	N	GLY	B	880	12.974	37.194	18.075	1.00	40.80

FIG. 5G

ATOM	395	CA	GLY	B	880	14.164	37.870	17.686	1.00	42.66
ATOM	396	C	GLY	B	880	14.499	39.226	18.185	1.00	43.75
ATOM	397	O	GLY	B	880	15.698	39.526	18.103	1.00	46.29
ATOM	398	N	HIS	B	881	13.580	40.053	18.637	1.00	42.86
ATOM	399	CA	HIS	B	881	13.759	41.403	19.105	1.00	43.65
ATOM	400	C	HIS	B	881	14.619	41.378	20.370	1.00	39.48
ATOM	401	O	HIS	B	881	15.539	42.203	20.446	1.00	43.05
ATOM	402	CB	HIS	B	881	12.417	42.127	19.236	1.00	47.39
ATOM	403	CG	HIS	B	881	11.628	42.051	20.490	1.00	50.98
ATOM	404	ND1	HIS	B	881	10.412	41.442	20.685	1.00	53.62
ATOM	405	CD2	HIS	B	881	11.944	42.576	21.711	1.00	53.62
ATOM	406	CE1	HIS	B	881	10.057	41.591	21.975	1.00	55.27
ATOM	407	NE2	HIS	B	881	10.966	42.286	22.647	1.00	55.05
ATOM	408	N	HIS	B	882	14.422	40.401	21.250	1.00	35.00
ATOM	409	CA	HIS	B	882	15.234	40.280	22.473	1.00	33.75
ATOM	410	C	HIS	B	882	16.695	40.394	22.053	1.00	29.63
ATOM	411	O	HIS	B	882	17.099	39.702	21.115	1.00	32.51
ATOM	412	CB	HIS	B	882	14.977	38.947	23.240	1.00	29.31
ATOM	413	CG	HIS	B	882	15.458	39.007	24.665	1.00	28.91
ATOM	414	ND1	HIS	B	882	16.739	38.861	25.208	1.00	28.25
ATOM	415	CD2	HIS	B	882	14.687	39.334	25.705	1.00	27.99
ATOM	416	CE1	HIS	B	882	16.623	39.049	26.523	1.00	28.98
ATOM	417	NE2	HIS	B	882	15.346	39.333	26.866	1.00	26.63
ATOM	418	N	PRO	B	883	17.468	41.252	22.659	1.00	31.32
ATOM	419	CA	PRO	B	883	18.882	41.398	22.375	1.00	31.40
ATOM	420	C	PRO	B	883	19.687	40.158	22.658	1.00	32.62
ATOM	421	O	PRO	B	883	20.700	39.965	21.941	1.00	36.70
ATOM	422	CB	PRO	B	883	19.206	42.672	23.123	1.00	30.55
ATOM	423	CG	PRO	B	883	18.433	42.543	24.437	1.00	33.27
ATOM	424	CD	PRO	B	883	17.096	42.064	23.858	1.00	31.21
ATOM	425	N	ASN	B	884	19.290	39.189	23.448	1.00	33.73
ATOM	426	CA	ASN	B	884	19.999	37.942	23.685	1.00	32.47
ATOM	427	C	ASN	B	884	19.496	36.811	22.823	1.00	34.37
ATOM	428	O	ASN	B	884	19.901	35.659	23.051	1.00	34.65
ATOM	429	CB	ASN	B	884	19.952	37.596	25.173	1.00	33.46
ATOM	430	CG	ASN	B	884	20.404	38.649	26.117	1.00	36.23
ATOM	431	OD1	ASN	B	884	20.011	39.181	27.122	1.00	37.73
ATOM	432	ND2	ASN	B	884	21.749	38.992	25.840	1.00	32.70
ATOM	433	N	ILE	B	885	18.623	37.014	21.825	1.00	32.48
ATOM	434	CA	ILE	B	885	18.185	36.032	20.859	1.00	34.12
ATOM	435	C	ILE	B	885	18.587	36.426	19.455	1.00	32.76
ATOM	436	O	ILE	B	885	18.359	37.539	18.982	1.00	33.37
ATOM	437	CB	ILE	B	885	16.662	35.743	21.004	1.00	33.83
ATOM	438	CG1	ILE	B	885	16.442	35.119	22.402	1.00	35.22
ATOM	439	CG2	ILE	B	885	16.088	34.847	19.922	1.00	33.58
ATOM	440	CD1	ILE	B	885	14.970	34.840	22.653	1.00	38.35
ATOM	441	N	ILE	B	886	19.261	35.557	18.697	1.00	34.99
ATOM	442	CA	ILE	B	886	19.694	35.965	17.333	1.00	37.58
ATOM	443	C	ILE	B	886	18.478	36.272	16.468	1.00	39.01
ATOM	444	O	ILE	B	886	17.526	35.459	16.453	1.00	38.20
ATOM	445	CB	ILE	B	886	20.693	34.967	16.752	1.00	38.15
ATOM	446	CG1	ILE	B	886	21.549	35.590	15.622	1.00	40.28
ATOM	447	CG2	ILE	B	886	19.985	33.776	16.206	1.00	38.96
ATOM	448	CD1	ILE	B	886	22.675	36.445	16.190	1.00	39.25
ATOM	449	N	ASN	B	887	18.472	37.380	15.731	1.00	38.67
ATOM	450	CA	ASN	B	887	17.268	37.824	15.016	1.00	40.23
ATOM	451	C	ASN	B	887	17.116	37.485	13.560	1.00	40.18

FIG. 5H

ATOM	452	O	ASN	B	887	18.061	37.480	12.780	1.00	41.35
ATOM	453	CB	ASN	B	887	17.153	39.347	15.231	1.00	40.41
ATOM	454	CG	ASN	B	887	15.888	39.999	14.697	1.00	40.25
ATOM	455	OD1	ASN	B	887	15.961	41.166	14.290	1.00	39.53
ATOM	456	ND2	ASN	B	887	14.746	39.340	14.692	1.00	38.70
ATOM	457	N	LEU	B	888	15.891	37.146	13.147	1.00	42.05
ATOM	458	CA	LEU	B	888	15.624	36.781	11.744	1.00	43.89
ATOM	459	C	LEU	B	888	15.501	38.053	10.900	1.00	44.52
ATOM	460	O	LEU	B	888	14.790	38.957	11.351	1.00	42.69
ATOM	461	CB	LEU	B	888	14.321	35.988	11.680	1.00	45.35
ATOM	462	CG	LEU	B	888	13.675	35.835	10.310	1.00	46.44
ATOM	463	CD1	LEU	B	888	14.617	35.185	9.322	1.00	47.08
ATOM	464	CD2	LEU	B	888	12.393	35.011	10.433	1.00	48.74
ATOM	465	N	LEU	B	889	16.221	38.160	9.785	1.00	46.33
ATOM	466	CA	LEU	B	889	16.106	39.377	9.004	1.00	48.96
ATOM	467	C	LEU	B	889	15.178	39.162	7.822	1.00	48.91
ATOM	468	O	LEU	B	889	14.331	40.055	7.642	1.00	52.61
ATOM	469	CB	LEU	B	889	17.407	40.091	8.621	1.00	52.03
ATOM	470	CG	LEU	B	889	18.022	40.806	9.850	1.00	54.44
ATOM	471	CD1	LEU	B	889	18.709	39.713	10.624	1.00	56.62
ATOM	472	CD2	LEU	B	889	19.053	41.862	9.535	1.00	56.92
ATOM	473	N	GLY	B	890	15.192	38.056	7.122	1.00	48.86
ATOM	474	CA	GLY	B	890	14.281	37.806	6.027	1.00	49.19
ATOM	475	C	GLY	B	890	14.348	36.393	5.478	1.00	51.62
ATOM	476	O	GLY	B	890	15.216	35.581	5.811	1.00	49.54
ATOM	477	N	ALA	B	891	13.367	36.080	4.619	1.00	52.67
ATOM	478	CA	ALA	B	891	13.339	34.779	3.956	1.00	55.84
ATOM	479	C	ALA	B	891	13.195	35.036	2.454	1.00	58.68
ATOM	480	O	ALA	B	891	12.782	36.128	2.056	1.00	60.04
ATOM	481	CB	ALA	B	891	12.292	33.826	4.471	1.00	54.13
ATOM	482	N	CYS	B	892	13.681	34.109	1.646	1.00	61.71
ATOM	483	CA	CYS	B	892	13.618	34.248	0.200	1.00	64.65
ATOM	484	C	CYS	B	892	13.505	32.847	-0.403	1.00	67.70
ATOM	485	O	CYS	B	892	14.279	31.955	-0.046	1.00	68.56
ATOM	486	CB	CYS	B	892	14.817	34.942	-0.412	1.00	63.99
ATOM	487	SG	CYS	B	892	14.859	34.973	-2.216	1.00	64.16
ATOM	488	N	GLU	B	893	12.506	32.682	-1.262	1.00	70.26
ATOM	489	CA	GLU	B	893	12.337	31.411	-1.965	1.00	72.47
ATOM	490	C	GLU	B	893	12.959	31.542	-3.354	1.00	72.44
ATOM	491	O	GLU	B	893	12.603	32.421	-4.134	1.00	72.20
ATOM	492	CB	GLU	B	893	10.873	30.991	-2.027	1.00	74.16
ATOM	493	CG	GLU	B	893	10.291	30.437	-0.736	1.00	76.17
ATOM	494	CD	GLU	B	893	8.789	30.210	-0.801	1.00	77.74
ATOM	495	OE1	GLU	B	893	8.126	30.906	-1.611	1.00	78.37
ATOM	496	OE2	GLU	B	893	8.230	29.357	-0.069	1.00	78.86
ATOM	497	N	HIS	B	894	13.922	30.697	-3.677	1.00	73.54
ATOM	498	CA	HIS	B	894	14.594	30.700	-4.977	1.00	74.67
ATOM	499	C	HIS	B	894	14.847	29.255	-5.401	1.00	74.91
ATOM	500	O	HIS	B	894	15.025	28.386	-4.542	1.00	74.35
ATOM	501	CB	HIS	B	894	15.857	31.531	-4.919	1.00	75.48
ATOM	502	CG	HIS	B	894	16.558	31.697	-6.225	1.00	76.90
ATOM	503	ND1	HIS	B	894	17.369	30.719	-6.752	1.00	77.63
ATOM	504	CD2	HIS	B	894	16.587	32.733	-7.097	1.00	77.64
ATOM	505	CE1	HIS	B	894	17.880	31.150	-7.893	1.00	78.14
ATOM	506	NE2	HIS	B	894	17.433	32.377	-8.119	1.00	77.87
ATOM	507	N	ARG	B	895	14.774	28.959	-6.699	1.00	74.84
ATOM	508	CA	ARG	B	895	14.865	27.593	-7.214	1.00	73.98

FIG. 5I

ATOM	509	C	ARG	B	895	14.001	26.742	-6.281	1.00	74.16
ATOM	510	O	ARG	B	895	12.911	27.249	-5.967	1.00	74.67
ATOM	511	CB	ARG	B	895	16.262	27.053	-7.367	1.00	74.14
ATOM	512	N	GLY	B	896	14.429	25.597	-5.769	1.00	73.62
ATOM	513	CA	GLY	B	896	13.554	24.843	-4.878	1.00	74.58
ATOM	514	C	GLY	B	896	13.801	24.946	-3.383	1.00	75.31
ATOM	515	O	GLY	B	896	13.362	24.085	-2.599	1.00	74.62
ATOM	516	N	TYR	B	897	14.568	25.958	-2.952	1.00	75.55
ATOM	517	CA	TYR	B	897	14.937	26.107	-1.551	1.00	75.78
ATOM	518	C	TYR	B	897	14.498	27.408	-0.882	1.00	73.41
ATOM	519	O	TYR	B	897	14.296	28.420	-1.548	1.00	73.50
ATOM	520	CB	TYR	B	897	16.466	26.038	-1.444	1.00	78.25
ATOM	521	CG	TYR	B	897	17.225	24.811	-1.836	1.00	80.53
ATOM	522	CD1	TYR	B	897	17.259	24.356	-3.145	1.00	81.37
ATOM	523	CD2	TYR	B	897	17.982	24.114	-0.898	1.00	81.11
ATOM	524	CE1	TYR	B	897	17.983	23.232	-3.498	1.00	82.95
ATOM	525	CE2	TYR	B	897	18.712	22.994	-1.247	1.00	82.00
ATOM	526	CZ	TYR	B	897	18.723	22.542	-2.554	1.00	82.42
ATOM	527	N	LEU	B	898	14.434	27.417	0.450	1.00	70.37
ATOM	528	CA	LEU	B	898	14.132	28.667	1.172	1.00	68.25
ATOM	529	C	LEU	B	898	15.407	29.218	1.794	1.00	66.94
ATOM	530	O	LEU	B	898	16.271	28.530	2.340	1.00	67.22
ATOM	531	CB	LEU	B	898	12.957	28.443	2.089	1.00	67.63
ATOM	532	CG	LEU	B	898	12.979	28.839	3.549	1.00	66.92
ATOM	533	CD1	LEU	B	898	11.612	29.212	4.063	1.00	67.30
ATOM	534	CD2	LEU	B	898	13.492	27.667	4.393	1.00	67.72
ATOM	535	N	TYR	B	899	15.648	30.512	1.585	1.00	65.23
ATOM	536	CA	TYR	B	899	16.871	31.191	2.019	1.00	61.95
ATOM	537	C	TYR	B	899	16.601	32.001	3.262	1.00	60.81
ATOM	538	O	TYR	B	899	15.646	32.797	3.247	1.00	61.40
ATOM	539	CB	TYR	B	899	17.291	31.923	0.733	1.00	62.33
ATOM	540	CG	TYR	B	899	17.999	31.028	-0.267	1.00	63.29
ATOM	541	CD1	TYR	B	899	17.347	30.060	-1.018	1.00	63.92
ATOM	542	CD2	TYR	B	899	19.373	31.154	-0.439	1.00	63.86
ATOM	543	CE1	TYR	B	899	18.025	29.235	-1.897	1.00	64.75
ATOM	544	CE2	TYR	B	899	20.078	30.345	-1.317	1.00	64.65
ATOM	545	CZ	TYR	B	899	19.395	29.384	-2.041	1.00	65.94
ATOM	546	OH	TYR	B	899	20.089	28.577	-2.918	1.00	66.41
ATOM	547	N	LEU	B	900	17.269	31.750	4.397	1.00	56.58
ATOM	548	CA	LEU	B	900	17.006	32.506	5.625	1.00	52.46
ATOM	549	C	LEU	B	900	18.209	33.421	5.892	1.00	50.69
ATOM	550	O	LEU	B	900	19.359	33.002	5.834	1.00	49.63
ATOM	551	CB	LEU	B	900	16.742	31.664	6.859	1.00	52.94
ATOM	552	CG	LEU	B	900	15.786	30.472	6.845	1.00	53.46
ATOM	553	CD1	LEU	B	900	16.449	29.204	6.312	1.00	53.02
ATOM	554	CD2	LEU	B	900	15.211	30.153	8.224	1.00	53.76
ATOM	555	N	ALA	B	901	17.923	34.696	6.093	1.00	48.07
ATOM	556	CA	ALA	B	901	18.972	35.699	6.337	1.00	44.87
ATOM	557	C	ALA	B	901	18.893	36.119	7.800	1.00	42.43
ATOM	558	O	ALA	B	901	17.895	36.689	8.253	1.00	41.24
ATOM	559	CB	ALA	B	901	18.777	36.899	5.429	1.00	43.13
ATOM	560	N	ILE	B	902	19.919	35.717	8.532	1.00	42.59
ATOM	561	CA	ILE	B	902	20.012	35.929	9.979	1.00	40.02
ATOM	562	C	ILE	B	902	20.926	37.088	10.334	1.00	40.16
ATOM	563	O	ILE	B	902	21.844	37.413	9.586	1.00	41.22
ATOM	564	CB	ILE	B	902	20.561	34.648	10.635	1.00	39.22
ATOM	565	CG1	ILE	B	902	19.781	33.405	10.190	1.00	41.67

FIG. 5J

ATOM	566	CG2	ILE	B	902	20.538	34.742	12.152	1.00	38.02
ATOM	567	CD1	ILE	B	902	18.288	33.542	10.392	1.00	44.70
ATOM	568	N	GLU	B	903	20.702	37.692	11.498	1.00	38.24
ATOM	569	CA	GLU	B	903	21.487	38.756	12.058	1.00	36.51
ATOM	570	C	GLU	B	903	22.929	38.231	12.121	1.00	37.45
ATOM	571	O	GLU	B	903	23.188	37.096	12.569	1.00	37.05
ATOM	572	CB	GLU	B	903	20.984	39.024	13.484	1.00	36.53
ATOM	573	CG	GLU	B	903	21.936	39.865	14.343	1.00	39.44
ATOM	574	CD	GLU	B	903	21.384	40.070	15.735	1.00	40.57
ATOM	575	OE1	GLU	B	903	21.848	40.909	16.534	1.00	39.27
ATOM	576	OE2	GLU	B	903	20.387	39.361	16.065	1.00	39.59
ATOM	577	N	TYR	B	904	23.817	39.039	11.558	1.00	36.26
ATOM	578	CA	TYR	B	904	25.236	38.729	11.507	1.00	38.11
ATOM	579	C	TYR	B	904	25.928	39.016	12.842	1.00	36.13
ATOM	580	O	TYR	B	904	25.810	40.085	13.447	1.00	36.04
ATOM	581	CB	TYR	B	904	25.870	39.456	10.293	1.00	38.03
ATOM	582	CG	TYR	B	904	27.340	39.121	10.159	1.00	39.56
ATOM	583	CD1	TYR	B	904	27.790	37.827	9.900	1.00	40.02
ATOM	584	CD2	TYR	B	904	28.296	40.122	10.364	1.00	39.80
ATOM	585	CE1	TYR	B	904	29.154	37.532	9.822	1.00	40.07
ATOM	586	CE2	TYR	B	904	29.641	39.846	10.258	1.00	39.30
ATOM	587	CZ	TYR	B	904	30.043	38.571	9.994	1.00	38.67
ATOM	588	OH	TYR	B	904	31.395	38.341	9.943	1.00	42.02
ATOM	589	N	ALA	B	905	26.565	37.994	13.427	1.00	33.70
ATOM	590	CA	ALA	B	905	27.351	38.148	14.629	1.00	34.04
ATOM	591	C	ALA	B	905	28.807	38.331	14.173	1.00	34.59
ATOM	592	O	ALA	B	905	29.422	37.413	13.631	1.00	34.61
ATOM	593	CB	ALA	B	905	27.272	36.924	15.544	1.00	31.52
ATOM	594	N	PRO	B	906	29.362	39.523	14.313	1.00	37.23
ATOM	595	CA	PRO	B	906	30.702	39.735	13.790	1.00	36.90
ATOM	596	C	PRO	B	906	31.854	39.167	14.554	1.00	37.30
ATOM	597	O	PRO	B	906	32.998	39.226	14.071	1.00	37.05
ATOM	598	CB	PRO	B	906	30.757	41.248	13.601	1.00	38.72
ATOM	599	CG	PRO	B	906	29.641	41.840	14.378	1.00	39.46
ATOM	600	CD	PRO	B	906	28.736	40.738	14.854	1.00	35.60
ATOM	601	N	HIS	B	907	31.720	38.652	15.767	1.00	35.76
ATOM	602	CA	HIS	B	907	32.810	38.072	16.515	1.00	34.45
ATOM	603	C	HIS	B	907	32.768	36.551	16.532	1.00	33.29
ATOM	604	O	HIS	B	907	33.420	36.044	17.429	1.00	36.68
ATOM	605	CB	HIS	B	907	32.793	38.614	17.971	1.00	32.90
ATOM	606	CG	HIS	B	907	32.706	40.082	17.966	1.00	33.20
ATOM	607	ND1	HIS	B	907	33.802	40.846	17.590	1.00	35.03
ATOM	608	CD2	HIS	B	907	31.727	40.985	18.200	1.00	31.98
ATOM	609	CE1	HIS	B	907	33.497	42.128	17.610	1.00	33.06
ATOM	610	NE2	HIS	B	907	32.241	42.248	18.017	1.00	33.02
ATOM	611	N	GLY	B	908	32.021	35.804	15.757	1.00	30.48
ATOM	612	CA	GLY	B	908	32.010	34.380	15.765	1.00	32.68
ATOM	613	C	GLY	B	908	31.084	33.774	16.838	1.00	31.58
ATOM	614	O	GLY	B	908	30.218	34.407	17.431	1.00	28.30
ATOM	615	N	ASN	B	909	31.300	32.477	17.068	1.00	27.49
ATOM	616	CA	ASN	B	909	30.550	31.793	18.108	1.00	24.09
ATOM	617	C	ASN	B	909	31.321	32.036	19.407	1.00	25.93
ATOM	618	O	ASN	B	909	32.485	32.498	19.367	1.00	28.49
ATOM	619	CB	ASN	B	909	30.241	30.343	17.894	1.00	26.09
ATOM	620	CG	ASN	B	909	31.306	29.286	17.946	1.00	28.79
ATOM	621	OD1	ASN	B	909	31.088	28.055	17.867	1.00	30.89
ATOM	622	ND2	ASN	B	909	32.526	29.772	18.045	1.00	25.36

ATOM	623	N	LEU	B	910	30.721	31.746	20.545	1.00 23.98
ATOM	624	CA	LEU	B	910	31.369	32.013	21.809	1.00 24.27
ATOM	625	C	LEU	B	910	32.494	31.025	22.149	1.00 28.34
ATOM	626	O	LEU	B	910	33.475	31.482	22.740	1.00 28.22
ATOM	627	CB	LEU	B	910	30.268	31.885	22.850	1.00 22.33
ATOM	628	CG	LEU	B	910	30.701	31.957	24.327	1.00 23.69
ATOM	629	CD1	LEU	B	910	31.394	33.213	24.683	1.00 22.29
ATOM	630	CD2	LEU	B	910	29.417	31.790	25.166	1.00 21.67
ATOM	631	N	LEU	B	911	32.290	29.750	21.805	1.00 27.95
ATOM	632	CA	LEU	B	911	33.380	28.801	22.034	1.00 25.73
ATOM	633	C	LEU	B	911	34.638	29.295	21.337	1.00 27.49
ATOM	634	O	LEU	B	911	35.676	29.359	22.043	1.00 26.42
ATOM	635	CB	LEU	B	911	33.003	27.396	21.533	1.00 27.05
ATOM	636	CG	LEU	B	911	34.062	26.292	21.771	1.00 25.84
ATOM	637	CD1	LEU	B	911	34.319	26.301	23.302	1.00 20.85
ATOM	638	CD2	LEU	B	911	33.505	24.899	21.410	1.00 23.88
ATOM	639	N	ASP	B	912	34.686	29.509	20.034	1.00 27.48
ATOM	640	CA	ASP	B	912	35.832	30.077	19.341	1.00 30.26
ATOM	641	C	ASP	B	912	36.323	31.426	19.869	1.00 31.88
ATOM	642	O	ASP	B	912	37.540	31.676	19.938	1.00 29.65
ATOM	643	CB	ASP	B	912	35.557	30.313	17.848	1.00 30.57
ATOM	644	CG	ASP	B	912	35.339	29.102	16.995	1.00 34.53
ATOM	645	OD1	ASP	B	912	34.882	29.274	15.841	1.00 37.84
ATOM	646	OD2	ASP	B	912	35.663	27.975	17.416	1.00 37.21
ATOM	647	N	PHE	B	913	35.440	32.298	20.355	1.00 31.78
ATOM	648	CA	PHE	B	913	35.763	33.564	20.967	1.00 29.21
ATOM	649	C	PHE	B	913	36.507	33.319	22.291	1.00 30.28
ATOM	650	O	PHE	B	913	37.612	33.931	22.463	1.00 27.63
ATOM	651	CB	PHE	B	913	34.591	34.492	21.208	1.00 27.45
ATOM	652	CG	PHE	B	913	34.831	35.958	21.499	1.00 29.93
ATOM	653	CD1	PHE	B	913	35.060	36.840	20.461	1.00 28.75
ATOM	654	CD2	PHE	B	913	34.910	36.415	22.816	1.00 27.43
ATOM	655	CE1	PHE	B	913	35.313	38.202	20.715	1.00 28.06
ATOM	656	CE2	PHE	B	913	35.188	37.763	23.068	1.00 29.46
ATOM	657	CZ	PHE	B	913	35.379	38.643	22.029	1.00 28.47
ATOM	658	N	LEU	B	914	36.054	32.404	23.151	1.00 26.55
ATOM	659	CA	LEU	B	914	36.844	32.188	24.365	1.00 31.20
ATOM	660	C	LEU	B	914	38.154	31.425	24.075	1.00 30.42
ATOM	661	O	LEU	B	914	39.065	31.539	24.890	1.00 29.64
ATOM	662	CB	LEU	B	914	36.133	31.379	25.440	1.00 32.99
ATOM	663	CG	LEU	B	914	34.718	31.897	25.858	1.00 32.39
ATOM	664	CD1	LEU	B	914	33.745	30.794	26.190	1.00 31.43
ATOM	665	CD2	LEU	B	914	34.981	32.805	27.062	1.00 27.44
ATOM	666	N	ARG	B	915	38.196	30.595	23.029	1.00 28.43
ATOM	667	CA	ARG	B	915	39.414	29.824	22.755	1.00 29.31
ATOM	668	C	ARG	B	915	40.498	30.753	22.149	1.00 32.00
ATOM	669	O	ARG	B	915	41.692	30.583	22.478	1.00 33.32
ATOM	670	CB	ARG	B	915	39.157	28.572	21.911	1.00 25.22
ATOM	671	CG	ARG	B	915	38.723	27.348	22.800	1.00 24.37
ATOM	672	CD	ARG	B	915	38.161	26.209	21.957	1.00 24.35
ATOM	673	NE	ARG	B	915	37.642	25.132	22.889	1.00 26.89
ATOM	674	CZ	ARG	B	915	37.100	24.031	22.346	1.00 25.09
ATOM	675	NH1	ARG	B	915	37.054	23.901	21.016	1.00 24.19
ATOM	676	NH2	ARG	B	915	36.588	23.111	23.194	1.00 23.94
ATOM	677	N	LYS	B	916	40.164	31.751	21.372	1.00 34.12
ATOM	678	CA	LYS	B	916	40.980	32.736	20.705	1.00 35.63
ATOM	679	C	LYS	B	916	41.664	33.693	21.683	1.00 36.01

FIG. 5L

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ATOM    680  O   LYS B 916      42.752  34.252  21.536  1.00 36.61
ATOM    681  CB  LYS B 916      40.287  33.552  19.615  1.00 34.37
ATOM    682  CG  LYS B 916      40.129  32.825  18.298  1.00 42.16
ATOM    683  CD  LYS B 916      39.443  33.575  17.172  1.00 44.43
ATOM    684  CE  LYS B 916      38.756  32.732  16.114  1.00 47.47
ATOM    685  NZ  LYS B 916      37.371  33.261  15.814  1.00 51.77
ATOM    686  N   SER B 917      40.991  33.857  22.786  1.00 33.46
ATOM    687  CA  SER B 917      41.419  34.647  23.937  1.00 32.01
ATOM    688  C   SER B 917      42.545  34.012  24.721  1.00 32.62
ATOM    689  O   SER B 917      43.188  34.725  25.520  1.00 27.96
ATOM    690  CB  SER B 917      40.117  34.800  24.689  1.00 31.09
ATOM    691  OG  SER B 917      40.057  34.497  26.054  1.00 33.24
ATOM    692  N   ARG B 918      42.926  33.735  24.574  1.00 33.26
ATOM    693  CA  ARG B 918      43.911  33.087  25.401  1.00 29.88
ATOM    694  C   ARG B 918      45.341  33.471  24.927  1.00 33.33
ATOM    695  O   ARG B 918      46.072  31.782  24.226  1.00 34.36
ATOM    696  CB  ARG B 918      43.750  30.570  25.487  1.00 30.84
ATOM    697  CG  ARG B 918      42.350  30.118  25.969  1.00 31.53
ATOM    698  CD  ARG B 918      42.301  28.655  26.234  1.00 31.59
ATOM    699  NE  ARG B 918      41.373  27.771  26.776  1.00 30.40
ATOM    700  CZ  ARG B 918      41.314  26.510  27.146  1.00 27.78
ATOM    701  NH1 ARG B 918      42.579  25.901  27.032  1.00 24.30
ATOM    702  NH2 ARG B 918      40.359  25.804  27.635  1.00 24.57
ATOM    703  N   VAL B 919      45.792  33.639  25.388  1.00 29.19
ATOM    704  CA  VAL B 919      46.914  34.362  24.991  1.00 31.89
ATOM    705  C   VAL B 919      48.324  33.779  25.390  1.00 33.48
ATOM    706  O   VAL B 919      49.318  34.428  25.239  1.00 42.15
ATOM    707  CB  VAL B 919      47.064  35.854  25.366  1.00 30.88
ATOM    708  CG1 VAL B 919      46.027  36.669  24.602  1.00 34.82
ATOM    709  CG2 VAL B 919      46.881  36.061  26.852  1.00 31.88
ATOM    710  N   LEU B 920      48.272  32.609  25.986  1.00 31.42
ATOM    711  CA  LEU B 920      49.386  31.803  26.310  1.00 32.43
ATOM    712  C   LEU B 920      49.646  30.949  25.049  1.00 33.59
ATOM    713  O   LEU B 920      50.874  30.754  24.757  1.00 34.43
ATOM    714  CB  LEU B 920      49.363  30.892  27.516  1.00 26.98
ATOM    715  CG  LEU B 920      49.473  31.646  28.827  1.00 28.45
ATOM    716  CD1 LEU B 920      49.060  30.712  29.911  1.00 24.11
ATOM    717  CD2 LEU B 920      50.899  32.259  29.084  1.00 24.38
ATOM    718  N   GLU B 921      48.560  30.587  24.414  1.00 33.03
ATOM    719  CA  GLU B 921      48.691  29.839  23.163  1.00 34.88
ATOM    720  C   GLU B 921      48.686  30.741  21.960  1.00 36.44
ATOM    721  O   GLU B 921      49.468  30.532  21.028  1.00 37.60
ATOM    722  CB  GLU B 921      47.526  28.797  23.034  1.00 36.48
ATOM    723  CG  GLU B 921      47.367  28.228  21.636  1.00 39.16
ATOM    724  CD  GLU B 921      46.213  27.255  21.414  1.00 43.37
ATOM    725  OE1 GLU B 921      45.489  26.854  22.357  1.00 41.90
ATOM    726  OE2 GLU B 921      46.044  26.848  20.222  1.00 42.19
ATOM    727  N   THR B 922      47.772  31.738  21.886  1.00 33.22
ATOM    728  CA  THR B 922      47.684  32.482  20.652  1.00 33.16
ATOM    729  C   THR B 922      48.566  33.711  20.605  1.00 33.32
ATOM    730  O   THR B 922      48.787  34.124  19.452  1.00 33.82
ATOM    731  CB  THR B 922      46.212  32.897  20.346  1.00 33.96
ATOM    732  OG1 THR B 922      45.814  33.744  21.415  1.00 33.38
ATOM    733  CG2 THR B 922      45.288  31.667  20.363  1.00 35.79
ATOM    734  N   ASP B 923      49.134  34.252  21.645  1.00 34.17
ATOM    735  CA  ASP B 923      50.099  35.410  21.445  1.00 33.90
ATOM    736  C   ASP B 923      50.855  35.464  22.736  1.00 31.06
```

FIG. 5M

ATOM	737	O	ASP	B	923	50.593	36.342	23.567	1.00	27.46
ATOM	738	CB	ASP	B	923	49.307	36.710	21.268	1.00	37.04
ATOM	739	CG	ASP	B	923	50.153	37.937	20.960	1.00	41.38
ATOM	740	OD1	ASP	B	923	49.577	39.035	20.699	1.00	39.51
ATOM	741	OD2	ASP	B	923	51.412	37.813	20.986	1.00	38.37
ATOM	742	N	PRO	B	924	51.732	34.505	23.057	1.00	30.87
ATOM	743	CA	PRO	B	924	52.373	34.348	24.339	1.00	29.10
ATOM	744	C	PRO	B	924	53.219	35.487	24.884	1.00	30.48
ATOM	745	O	PRO	B	924	53.451	35.658	26.081	1.00	36.16
ATOM	746	CB	PRO	B	924	53.266	33.088	24.160	1.00	29.12
ATOM	747	CG	PRO	B	924	53.404	32.976	22.696	1.00	30.23
ATOM	748	CD	PRO	B	924	52.076	33.382	22.137	1.00	31.39
ATOM	749	N	ALA	B	925	53.613	36.368	24.008	1.00	26.00
ATOM	750	CA	ALA	B	925	54.366	37.598	24.150	1.00	32.47
ATOM	751	C	ALA	B	925	53.543	38.653	24.869	1.00	29.57
ATOM	752	O	ALA	B	925	53.787	39.195	25.935	1.00	30.49
ATOM	753	CB	ALA	B	925	54.773	38.221	22.799	1.00	31.57
ATOM	754	N	PHE	B	926	52.319	38.825	24.295	1.00	29.73
ATOM	755	CA	PHE	B	926	51.269	39.710	24.838	1.00	29.93
ATOM	756	C	PHE	B	926	51.056	39.489	26.342	1.00	26.49
ATOM	757	O	PHE	B	926	50.877	40.391	27.189	1.00	33.60
ATOM	758	CB	PHE	B	926	49.990	39.510	24.004	1.00	33.75
ATOM	759	CG	PHE	B	926	48.853	40.282	24.610	1.00	35.41
ATOM	760	CD1	PHE	B	926	48.530	41.563	24.201	1.00	35.32
ATOM	761	CD2	PHE	B	926	48.148	39.708	25.665	1.00	35.43
ATOM	762	CE1	PHE	B	926	47.510	42.237	24.860	1.00	37.62
ATOM	763	CE2	PHE	B	926	47.135	40.390	26.312	1.00	40.82
ATOM	764	CZ	PHE	B	926	46.803	41.649	25.884	1.00	37.83
ATOM	765	N	ALA	B	927	50.917	38.202	26.616	1.00	30.01
ATOM	766	CA	ALA	B	927	50.632	37.486	27.815	1.00	28.56
ATOM	767	C	ALA	B	927	51.656	37.637	28.900	1.00	29.51
ATOM	768	O	ALA	B	927	51.289	37.839	30.056	1.00	30.25
ATOM	769	CB	ALA	B	927	50.513	35.973	27.565	1.00	32.88
ATOM	770	N	ILE	B	928	52.948	37.452	28.535	1.00	31.84
ATOM	771	CA	ILE	B	928	54.019	37.696	29.494	1.00	33.06
ATOM	772	C	ILE	B	928	54.111	39.221	29.662	1.00	31.39
ATOM	773	O	ILE	B	928	54.206	39.681	30.804	1.00	32.12
ATOM	774	CB	ILE	B	928	55.354	37.042	29.050	1.00	34.86
ATOM	775	CG1	ILE	B	928	56.448	37.311	30.077	1.00	36.35
ATOM	776	CG2	ILE	B	928	55.833	37.483	27.689	1.00	36.48
ATOM	777	CD1	ILE	B	928	56.235	36.372	31.274	1.00	40.48
ATOM	778	N	ALA	B	929	53.998	40.026	28.623	1.00	32.07
ATOM	779	CA	ALA	B	929	54.114	41.493	28.884	1.00	35.07
ATOM	780	C	ALA	B	929	52.935	42.038	29.650	1.00	32.88
ATOM	781	O	ALA	B	929	53.152	42.885	30.515	1.00	32.96
ATOM	782	CB	ALA	B	929	54.276	42.286	27.584	1.00	38.44
ATOM	783	N	ASN	B	930	51.737	41.363	29.538	1.00	32.01
ATOM	784	CA	ASN	B	930	50.624	41.923	30.307	1.00	32.62
ATOM	785	C	ASN	B	930	50.458	41.157	31.604	1.00	32.33
ATOM	786	O	ASN	B	930	49.549	41.509	32.315	1.00	30.28
ATOM	787	CB	ASN	B	930	49.305	41.975	29.564	1.00	30.21
ATOM	788	CG	ASN	B	930	49.462	43.166	28.612	1.00	34.16
ATOM	789	OD1	ASN	B	930	49.104	44.224	29.139	1.00	35.09
ATOM	790	ND2	ASN	B	930	49.997	42.925	27.434	1.00	33.29
ATOM	791	N	SER	B	931	51.284	40.126	31.740	1.00	31.40
ATOM	792	CA	SER	B	931	51.064	39.195	32.863	1.00	34.73
ATOM	793	C	SER	B	931	49.616	38.647	32.909	1.00	31.81

FIG. 5N

ATOM	794	O	SER	B	931	48.946	38.522	33.960	1.00	28.51
ATOM	795	CB	SER	B	931	51.539	39.966	34.083	1.00	36.38
ATOM	796	OG	SER	B	931	51.372	39.137	35.239	1.00	44.81
ATOM	797	N	THR	B	932	49.066	38.367	31.708	1.00	31.32
ATOM	798	CA	THR	B	932	47.681	37.822	31.741	1.00	33.33
ATOM	799	C	THR	B	932	47.532	36.490	31.036	1.00	31.10
ATOM	800	O	THR	B	932	48.276	36.141	30.127	1.00	30.68
ATOM	801	CB	THR	B	932	46.678	38.870	31.263	1.00	33.87
ATOM	802	OG1	THR	B	932	45.316	38.426	31.576	1.00	33.49
ATOM	803	CG2	THR	B	932	46.692	39.109	29.757	1.00	33.71
ATOM	804	N	ALA	B	933	46.529	35.668	31.389	1.00	31.61
ATOM	805	CA	ALA	B	933	46.226	34.431	30.705	1.00	29.07
ATOM	806	C	ALA	B	933	45.091	34.589	29.655	1.00	30.40
ATOM	807	O	ALA	B	933	44.908	33.676	28.853	1.00	28.66
ATOM	808	CB	ALA	B	933	45.737	33.378	31.703	1.00	27.24
ATOM	809	N	SER	B	934	44.450	35.779	29.587	1.00	26.77
ATOM	810	CA	SER	B	934	43.413	36.013	28.587	1.00	28.62
ATOM	811	C	SER	B	934	43.192	37.464	28.195	1.00	27.31
ATOM	812	O	SER	B	934	43.323	38.417	28.980	1.00	27.55
ATOM	813	CB	SER	B	934	42.064	35.455	29.162	1.00	26.81
ATOM	814	OG	SER	B	934	40.981	35.744	28.323	1.00	27.56
ATOM	815	N	THR	B	935	42.820	37.745	26.944	1.00	27.99
ATOM	816	CA	THR	B	935	42.439	39.110	26.578	1.00	29.68
ATOM	817	C	THR	B	935	41.160	39.524	27.282	1.00	31.68
ATOM	818	O	THR	B	935	40.842	40.718	27.320	1.00	33.62
ATOM	819	CB	THR	B	935	42.242	39.350	25.075	1.00	28.76
ATOM	820	OG1	THR	B	935	41.506	38.262	24.505	1.00	29.66
ATOM	821	CG2	THR	B	935	43.525	39.478	24.287	1.00	30.80
ATOM	822	N	LEU	B	936	40.343	38.579	27.771	1.00	30.00
ATOM	823	CA	LEU	B	936	39.018	38.902	28.323	1.00	31.45
ATOM	824	C	LEU	B	936	39.137	39.093	29.820	1.00	29.86
ATOM	825	O	LEU	B	936	39.947	38.339	30.364	1.00	28.85
ATOM	826	CB	LEU	B	936	38.171	37.634	28.127	1.00	35.21
ATOM	827	CG	LEU	B	936	37.312	37.342	26.944	1.00	38.52
ATOM	828	CD1	LEU	B	936	37.602	38.053	25.641	1.00	42.04
ATOM	829	CD2	LEU	B	936	37.181	35.833	26.689	1.00	40.21
ATOM	830	N	SER	B	937	38.381	39.888	30.508	1.00	28.66
ATOM	831	CA	SER	B	937	38.427	39.976	31.975	1.00	27.30
ATOM	832	C	SER	B	937	37.373	39.107	32.612	1.00	25.12
ATOM	833	O	SER	B	937	36.444	38.641	31.960	1.00	29.26
ATOM	834	CB	SER	B	937	38.164	41.408	32.478	1.00	28.29
ATOM	835	OG	SER	B	937	36.753	41.746	32.275	1.00	26.99
ATOM	836	N	SER	B	938	37.382	38.946	33.936	1.00	23.75
ATOM	837	CA	SER	B	938	36.444	38.301	34.738	1.00	25.14
ATOM	838	C	SER	B	938	34.982	38.781	34.508	1.00	29.67
ATOM	839	O	SER	B	938	33.973	38.052	34.324	1.00	28.12
ATOM	840	CB	SER	B	938	36.842	38.693	36.180	1.00	25.42
ATOM	841	OG	SER	B	938	35.935	37.879	36.971	1.00	31.24
ATOM	842	N	GLN	B	939	34.834	40.109	34.487	1.00	27.93
ATOM	843	CA	GLN	B	939	33.576	40.797	34.290	1.00	30.16
ATOM	844	C	GLN	B	939	33.036	40.463	32.911	1.00	26.11
ATOM	845	O	GLN	B	939	31.840	40.271	32.714	1.00	28.65
ATOM	846	CB	GLN	B	939	33.784	42.330	34.312	1.00	33.19
ATOM	847	CG	GLN	B	939	33.442	43.229	35.457	1.00	40.59
ATOM	848	CD	GLN	B	939	32.130	43.133	36.180	1.00	39.70
ATOM	849	OE1	GLN	B	939	31.005	43.468	35.831	1.00	47.06
ATOM	850	NE2	GLN	B	939	32.185	42.646	37.424	1.00	42.39

FIG. 50

ATOM	851	N	GLN	B	940	33.893	40.437	31.879	1.00 28.10
ATOM	852	CA	GLN	B	940	33.294	39.992	30.590	1.00 26.42
ATOM	853	C	GLN	B	940	32.792	38.510	30.608	1.00 27.93
ATOM	854	O	GLN	B	940	31.699	38.213	30.003	1.00 24.42
ATOM	855	CB	GLN	B	940	34.237	40.315	29.474	1.00 28.32
ATOM	856	CG	GLN	B	940	33.821	39.728	28.138	1.00 30.12
ATOM	857	CD	GLN	B	940	32.714	40.351	27.341	1.00 32.84
ATOM	858	OE1	GLN	B	940	32.980	40.952	26.293	1.00 32.97
ATOM	859	NE2	GLN	B	940	31.444	40.215	27.742	1.00 32.92
ATOM	860	N	LEU	B	941	33.469	37.651	31.370	1.00 26.91
ATOM	861	CA	LEU	B	941	32.909	36.258	31.443	1.00 28.19
ATOM	862	C	LEU	B	941	31.569	36.301	32.198	1.00 29.57
ATOM	863	O	LEU	B	941	30.678	35.590	31.730	1.00 30.43
ATOM	864	CB	LEU	B	941	33.906	35.296	32.049	1.00 25.27
ATOM	865	CG	LEU	B	941	35.315	35.323	31.415	1.00 32.42
ATOM	866	CD1	LEU	B	941	36.323	34.485	32.227	1.00 31.29
ATOM	867	CD2	LEU	B	941	35.341	34.767	30.010	1.00 31.88
ATOM	868	N	LEU	B	942	31.450	37.064	33.293	1.00 30.31
ATOM	869	CA	LEU	B	942	30.167	37.145	33.968	1.00 32.16
ATOM	870	C	LEU	B	942	29.036	37.749	33.115	1.00 31.83
ATOM	871	O	LEU	B	942	27.922	37.185	33.174	1.00 33.88
ATOM	872	CB	LEU	B	942	30.243	37.957	35.236	1.00 31.72
ATOM	873	CG	LEU	B	942	31.083	37.434	36.382	1.00 33.04
ATOM	874	CD1	LEU	B	942	31.284	38.550	37.417	1.00 33.30
ATOM	875	CD2	LEU	B	942	30.573	36.187	36.999	1.00 35.60
ATOM	876	N	HIS	B	943	29.333	38.722	32.292	1.00 30.14
ATOM	877	CA	HIS	B	943	28.489	39.305	31.307	1.00 32.55
ATOM	878	C	HIS	B	943	27.988	38.261	30.293	1.00 33.04
ATOM	879	O	HIS	B	943	26.773	38.281	29.997	1.00 29.13
ATOM	880	CB	HIS	B	943	29.051	40.525	30.513	1.00 31.92
ATOM	881	CG	HIS	B	943	28.919	41.826	31.219	1.00 34.62
ATOM	882	ND1	HIS	B	943	29.954	42.688	31.481	1.00 36.03
ATOM	883	CD2	HIS	B	943	27.832	42.442	31.778	1.00 38.05
ATOM	884	CE1	HIS	B	943	29.547	43.737	32.168	1.00 35.60
ATOM	885	NE2	HIS	B	943	28.245	43.626	32.354	1.00 37.32
ATOM	886	N	PHE	B	944	28.860	37.419	29.710	1.00 30.43
ATOM	887	CA	PHE	B	944	28.322	36.430	28.793	1.00 30.42
ATOM	888	C	PHE	B	944	27.361	35.447	29.480	1.00 28.35
ATOM	889	O	PHE	B	944	26.297	35.095	28.948	1.00 27.55
ATOM	890	CB	PHE	B	944	29.414	35.601	28.129	1.00 29.40
ATOM	891	CG	PHE	B	944	30.259	36.326	27.143	1.00 28.28
ATOM	892	CD1	PHE	B	944	31.639	36.118	27.152	1.00 28.85
ATOM	893	CD2	PHE	B	944	29.764	37.193	26.200	1.00 27.36
ATOM	894	CE1	PHE	B	944	32.429	36.783	26.230	1.00 31.22
ATOM	895	CE2	PHE	B	944	30.528	37.861	25.279	1.00 30.76
ATOM	896	CZ	PHE	B	944	31.863	37.640	25.305	1.00 29.54
ATOM	897	N	ALA	B	945	27.661	35.064	30.707	1.00 28.20
ATOM	898	CA	ALA	B	945	26.737	34.232	31.526	1.00 27.06
ATOM	899	C	ALA	B	945	25.389	34.896	31.781	1.00 28.16
ATOM	900	O	ALA	B	945	24.305	34.272	31.603	1.00 29.72
ATOM	901	CB	ALA	B	945	27.424	33.982	32.882	1.00 22.24
ATOM	902	N	ALA	B	946	25.348	36.185	32.154	1.00 28.40
ATOM	903	CA	ALA	B	946	24.058	36.906	32.424	1.00 26.80
ATOM	904	C	ALA	B	946	23.326	37.071	31.128	1.00 26.73
ATOM	905	O	ALA	B	946	22.095	36.826	30.960	1.00 33.16
ATOM	906	CB	ALA	B	946	24.422	38.268	33.049	1.00 27.29
ATOM	907	N	ASP	B	947	24.021	37.501	30.077	1.00 25.12

FIG. 5P

ATOM	908	CA	ASP	B	947	23.361	37.562	28.793	1.00	27.64
ATOM	909	C	ASP	B	947	22.653	36.217	28.522	1.00	30.15
ATOM	910	O	ASP	B	947	21.423	36.331	28.285	1.00	32.77
ATOM	911	CB	ASP	B	947	24.158	37.947	27.594	1.00	32.32
ATOM	912	CG	ASP	B	947	24.798	39.318	27.538	1.00	37.39
ATOM	913	OD1	ASP	B	947	24.327	40.283	28.209	1.00	38.95
ATOM	914	OD2	ASP	B	947	25.817	39.462	26.816	1.00	38.99
ATOM	915	N	VAL	B	948	23.225	35.043	28.511	1.00	24.93
ATOM	916	CA	VAL	B	948	22.519	33.824	28.235	1.00	26.37
ATOM	917	C	VAL	B	948	21.319	33.657	29.150	1.00	26.38
ATOM	918	O	VAL	B	948	20.273	33.241	28.688	1.00	28.00
ATOM	919	CB	VAL	B	948	23.423	32.575	28.375	1.00	23.63
ATOM	920	CG1	VAL	B	948	22.711	31.247	28.218	1.00	28.41
ATOM	921	CG2	VAL	B	948	24.500	32.621	27.306	1.00	24.29
ATOM	922	N	ALA	B	949	21.496	33.853	30.472	1.00	25.90
ATOM	923	CA	ALA	B	949	20.489	33.633	31.449	1.00	24.76
ATOM	924	C	ALA	B	949	19.254	34.514	31.245	1.00	29.82
ATOM	925	O	ALA	B	949	18.125	33.995	31.478	1.00	29.12
ATOM	926	CB	ALA	B	949	21.105	33.945	32.833	1.00	21.23
ATOM	927	N	ARG	B	950	19.483	35.753	30.814	1.00	29.05
ATOM	928	CA	ARG	B	950	18.417	36.711	30.563	1.00	29.74
ATOM	929	C	ARG	B	950	17.681	36.245	29.315	1.00	30.35
ATOM	930	O	ARG	B	950	16.454	36.156	29.291	1.00	32.30
ATOM	931	CB	ARG	B	950	18.943	38.135	30.331	1.00	29.04
ATOM	932	CG	ARG	B	950	17.857	39.209	30.253	1.00	29.74
ATOM	933	CD	ARG	B	950	18.484	40.540	29.840	1.00	33.11
ATOM	934	NE	ARG	B	950	19.702	40.789	30.623	1.00	36.26
ATOM	935	CZ	ARG	B	950	20.973	41.064	30.349	1.00	36.47
ATOM	936	NH1	ARG	B	950	21.905	41.281	31.276	1.00	34.51
ATOM	937	NH2	ARG	B	950	21.378	41.083	29.088	1.00	37.31
ATOM	938	N	GLY	B	951	18.419	35.817	28.306	1.00	29.52
ATOM	939	CA	GLY	B	951	17.811	35.222	27.135	1.00	30.22
ATOM	940	C	GLY	B	951	16.981	34.005	27.518	1.00	31.96
ATOM	941	O	GLY	B	951	15.802	33.895	27.083	1.00	30.42
ATOM	942	N	MET	B	952	17.505	33.082	28.335	1.00	31.58
ATOM	943	CA	MET	B	952	16.833	31.858	28.668	1.00	31.52
ATOM	944	C	MET	B	952	15.593	32.060	29.545	1.00	31.14
ATOM	945	O	MET	B	952	14.692	31.277	29.453	1.00	32.05
ATOM	946	CB	MET	B	952	17.728	30.817	29.348	1.00	32.91
ATOM	947	CG	MET	B	952	18.601	29.963	28.470	1.00	28.12
ATOM	948	SD	MET	B	952	17.803	29.220	27.056	1.00	28.47
ATOM	949	CE	MET	B	952	16.601	28.118	27.850	1.00	24.09
ATOM	950	N	ASP	B	953	15.540	32.991	30.425	1.00	33.12
ATOM	951	CA	ASP	B	953	14.479	33.295	31.364	1.00	35.52
ATOM	952	C	ASP	B	953	13.331	33.873	30.536	1.00	34.51
ATOM	953	O	ASP	B	953	12.167	33.463	30.579	1.00	34.88
ATOM	954	CB	ASP	B	953	14.959	34.196	32.470	1.00	37.38
ATOM	955	CG	ASP	B	953	13.886	35.033	33.182	1.00	38.60
ATOM	956	OD1	ASP	B	953	13.235	34.579	34.136	1.00	38.16
ATOM	957	OD2	ASP	B	953	13.774	36.209	32.830	1.00	39.51
ATOM	958	N	TYR	B	954	13.741	34.680	29.561	1.00	34.22
ATOM	959	CA	TYR	B	954	12.764	35.208	28.602	1.00	33.92
ATOM	960	C	TYR	B	954	12.083	34.027	27.920	1.00	35.03
ATOM	961	O	TYR	B	954	10.854	33.911	27.879	1.00	33.83
ATOM	962	CB	TYR	B	954	13.457	36.158	27.672	1.00	36.04
ATOM	963	CG	TYR	B	954	12.621	36.621	26.523	1.00	40.14
ATOM	964	CD1	TYR	B	954	11.489	37.372	26.834	1.00	42.51

FIG. 5Q

ATOM	965	CD2	TYR	B	954	12.873	36.322	25.202	1.00	40.08
ATOM	966	CE1	TYR	B	954	10.587	37.819	25.869	1.00	45.13
ATOM	967	CE2	TYR	B	954	12.012	36.762	24.225	1.00	44.28
ATOM	968	CZ	TYR	B	954	10.893	37.541	24.548	1.00	45.99
ATOM	969	OH	TYR	B	954	10.043	37.968	23.564	1.00	46.72
ATOM	970	N	LEU	B	955	12.809	33.080	27.399	1.00	34.55
ATOM	971	CA	LEU	B	955	12.388	31.912	26.704	1.00	34.31
ATOM	972	C	LEU	B	955	11.690	30.956	27.654	1.00	32.95
ATOM	973	O	LEU	B	955	10.537	30.633	27.336	1.00	36.79
ATOM	974	CB	LEU	B	955	13.431	31.053	26.006	1.00	34.82
ATOM	975	CG	LEU	B	955	14.032	31.673	24.757	1.00	30.87
ATOM	976	CD1	LEU	B	955	15.304	30.976	24.341	1.00	31.55
ATOM	977	CD2	LEU	B	955	13.075	31.726	23.592	1.00	32.89
ATOM	978	N	SER	B	956	12.231	30.620	28.798	1.00	33.38
ATOM	979	CA	SER	B	956	11.489	29.672	29.609	1.00	34.02
ATOM	980	C	SER	B	956	10.214	30.243	30.247	1.00	34.18
ATOM	981	O	SER	B	956	9.393	29.419	30.652	1.00	30.24
ATOM	982	CB	SER	B	956	12.469	29.126	30.630	1.00	33.64
ATOM	983	OG	SER	B	956	12.613	30.134	31.586	1.00	37.17
ATOM	984	N	GLN	B	957	10.032	31.530	30.438	1.00	32.94
ATOM	985	CA	GLN	B	957	8.852	32.137	31.059	1.00	37.57
ATOM	986	C	GLN	B	957	7.675	32.048	30.084	1.00	36.65
ATOM	987	O	GLN	B	957	6.518	31.962	30.443	1.00	36.69
ATOM	988	CB	GLN	B	957	9.101	33.516	31.671	1.00	39.36
ATOM	989	CG	GLN	B	957	9.819	33.491	33.028	1.00	43.44
ATOM	990	CD	GLN	B	957	10.305	34.801	33.581	1.00	47.63
ATOM	991	OE1	GLN	B	957	10.420	35.138	34.789	1.00	48.94
ATOM	992	NE2	GLN	B	957	10.736	35.802	32.807	1.00	50.75
ATOM	993	N	LYS	B	958	7.937	31.933	28.792	1.00	37.29
ATOM	994	CA	LYS	B	958	7.068	31.649	27.696	1.00	36.90
ATOM	995	C	LYS	B	958	6.830	30.166	27.402	1.00	39.87
ATOM	996	O	LYS	B	958	6.248	29.735	26.407	1.00	41.16
ATOM	997	CB	LYS	B	958	7.554	32.393	26.439	1.00	40.75
ATOM	998	CG	LYS	B	958	7.237	33.882	26.545	1.00	42.57
ATOM	999	CD	LYS	B	958	7.853	34.666	25.399	1.00	44.52
ATOM	1000	CE	LYS	B	958	6.950	35.852	25.045	1.00	49.59
ATOM	1001	NZ	LYS	B	958	7.755	36.850	24.277	1.00	50.56
ATOM	1002	N	GLN	B	959	7.238	29.272	28.275	1.00	38.89
ATOM	1003	CA	GLN	B	959	7.191	27.826	28.340	1.00	39.77
ATOM	1004	C	GLN	B	959	7.985	27.154	27.246	1.00	36.45
ATOM	1005	O	GLN	B	959	7.889	25.977	26.904	1.00	34.64
ATOM	1006	CB	GLN	B	959	5.729	27.298	28.353	1.00	42.27
ATOM	1007	CG	GLN	B	959	5.062	27.411	29.706	1.00	47.02
ATOM	1008	CD	GLN	B	959	3.550	27.270	29.700	1.00	52.44
ATOM	1009	OE1	GLN	B	959	2.905	27.301	30.787	1.00	54.64
ATOM	1010	NE2	GLN	B	959	2.888	27.133	28.539	1.00	51.33
ATOM	1011	N	PHE	B	960	8.932	27.911	26.701	1.00	35.89
ATOM	1012	CA	PHE	B	960	9.764	27.490	25.601	1.00	34.12
ATOM	1013	C	PHE	B	960	11.017	26.758	26.168	1.00	34.10
ATOM	1014	O	PHE	B	960	11.310	27.045	27.320	1.00	36.77
ATOM	1015	CB	PHE	B	960	10.127	28.752	24.850	1.00	38.30
ATOM	1016	CG	PHE	B	960	9.381	29.131	23.626	1.00	37.64
ATOM	1017	CD1	PHE	B	960	8.691	30.350	23.577	1.00	39.17
ATOM	1018	CD2	PHE	B	960	9.322	28.313	22.534	1.00	37.83
ATOM	1019	CE1	PHE	B	960	7.970	30.753	22.460	1.00	36.50
ATOM	1020	CE2	PHE	B	960	8.612	28.711	21.415	1.00	38.89
ATOM	1021	CZ	PHE	B	960	7.938	29.930	21.372	1.00	38.28

FIG. 5R

```
ATOM   1022  N   ILE B 961      11.301  25.645  25.515  1.00 32.04
ATOM   1023  CA  ILE B 961      12.386  24.751  25.913  1.00 35.73
ATOM   1024  C   ILE B 961      13.444  24.628  24.815  1.00 35.82
ATOM   1025  O   ILE B 961      13.170  24.025  23.764  1.00 36.60
ATOM   1026  CB  ILE B 961      11.866  23.322  26.185  1.00 37.85
ATOM   1027  CG1 ILE B 961      10.658  23.219  27.079  1.00 39.27
ATOM   1028  CG2 ILE B 961      12.985  22.443  26.741  1.00 41.20
ATOM   1029  CD1 ILE B 961      10.666  23.505  28.545  1.00 39.36
ATOM   1030  N   HIS B 962      14.751  24.959  25.030  1.00 33.60
ATOM   1031  CA  HIS B 962      15.736  24.996  23.975  1.00 31.29
ATOM   1032  C   HIS B 962      16.435  23.705  23.604  1.00 30.82
ATOM   1033  O   HIS B 962      16.658  23.371  22.425  1.00 29.73
ATOM   1034  CB  HIS B 962      16.674  26.099  24.539  1.00 31.33
ATOM   1035  CG  HIS B 962      17.589  26.596  23.457  1.00 33.97
ATOM   1036  ND1 HIS B 962      17.135  26.808  22.169  1.00 33.33
ATOM   1037  CD2 HIS B 962      18.913  26.881  23.499  1.00 33.27
ATOM   1038  CE1 HIS B 962      18.200  27.242  21.492  1.00 35.73
ATOM   1039  NE2 HIS B 962      19.289  27.260  22.251  1.00 29.66
ATOM   1040  N   ARG B 963      16.968  23.006  24.598  1.00 30.47
ATOM   1041  CA  ARG B 963      17.746  21.769  24.471  1.00 33.00
ATOM   1042  C   ARG B 963      19.194  21.923  23.997  1.00 36.77
ATOM   1043  O   ARG B 963      19.889  20.887  24.004  1.00 39.62
ATOM   1044  CB  ARG B 963      17.204  20.679  23.551  1.00 32.77
ATOM   1045  CG  ARG B 963      15.815  20.172  23.935  1.00 31.62
ATOM   1046  CD  ARG B 963      15.128  19.404  22.847  1.00 31.53
ATOM   1047  NE  ARG B 963      15.025  19.871  21.521  1.00 33.88
ATOM   1048  CZ  ARG B 963      15.726  19.662  20.419  1.00 37.97
ATOM   1049  NH1 ARG B 963      16.808  18.841  20.421  1.00 37.50
ATOM   1050  NH2 ARG B 963      15.341  20.285  19.289  1.00 37.35
ATOM   1051  N   ASN B 964      19.655  23.009  23.398  1.00 36.17
ATOM   1052  CA  ASN B 964      20.974  23.021  22.816  1.00 38.69
ATOM   1053  C   ASN B 964      21.926  24.070  23.372  1.00 36.17
ATOM   1054  O   ASN B 964      22.772  24.513  22.610  1.00 37.84
ATOM   1055  CB  ASN B 964      20.798  23.344  21.298  1.00 41.85
ATOM   1056  CG  ASN B 964      20.079  22.173  20.634  1.00 46.78
ATOM   1057  OD1 ASN B 964      20.319  21.037  21.043  1.00 49.94
ATOM   1058  ND2 ASN B 964      19.184  22.496  19.688  1.00 48.13
ATOM   1059  N   LEU B 965      21.795  24.534  24.570  1.00 32.14
ATOM   1060  CA  LEU B 965      22.546  25.569  25.189  1.00 33.80
ATOM   1061  C   LEU B 965      23.994  25.064  25.398  1.00 36.44
ATOM   1062  O   LEU B 965      24.144  24.390  26.421  1.00 40.41
ATOM   1063  CB  LEU B 965      22.086  25.960  26.578  1.00 31.51
ATOM   1064  CG  LEU B 965      20.940  26.943  26.863  1.00 30.06
ATOM   1065  CD1 LEU B 965      20.731  26.975  28.363  1.00 26.70
ATOM   1066  CD2 LEU B 965      21.491  28.298  26.403  1.00 29.20
ATOM   1067  N   ALA B 966      24.919  25.275  24.490  1.00 31.71
ATOM   1068  CA  ALA B 966      26.340  24.956  24.701  1.00 29.62
ATOM   1069  C   ALA B 966      27.144  26.139  24.175  1.00 27.97
ATOM   1070  O   ALA B 966      26.676  26.823  23.232  1.00 24.99
ATOM   1071  CB  ALA B 966      26.737  23.681  23.960  1.00 24.98
ATOM   1072  N   ALA B 967      28.451  26.232  24.492  1.00 28.41
ATOM   1073  CA  ALA B 967      29.236  27.348  23.991  1.00 25.71
ATOM   1074  C   ALA B 967      29.357  27.432  22.481  1.00 28.11
ATOM   1075  O   ALA B 967      29.291  28.561  21.897  1.00 26.71
ATOM   1076  CB  ALA B 967      30.515  27.596  24.725  1.00 28.93
ATOM   1077  N   ARG B 968      29.406  26.364  21.727  1.00 30.03
ATOM   1078  CA  ARG B 968      29.407  26.477  20.257  1.00 30.09
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FIG. 5S

ATOM	1079	C	ARG	B	968	28.100	27.003	19.677	1.00 30.62
ATOM	1080	O	ARG	B	968	28.131	27.362	18.476	1.00 31.68
ATOM	1081	CB	ARG	B	968	29.753	25.111	19.610	1.00 29.15
ATOM	1082	CG	ARG	B	968	28.695	24.044	19.886	1.00 31.62
ATOM	1083	CD	ARG	B	968	28.941	22.658	19.226	1.00 35.47
ATOM	1084	NE	ARG	B	968	27.817	21.807	19.703	1.00 38.33
ATOM	1085	CZ	ARG	B	968	27.827	21.154	20.851	1.00 40.05
ATOM	1086	NH1	ARG	B	968	28.897	21.164	21.633	1.00 42.72
ATOM	1087	NH2	ARG	B	968	26.834	20.421	21.322	1.00 43.32
ATOM	1088	N	ASN	B	969	26.979	27.025	20.436	1.00 28.92
ATOM	1089	CA	ASN	B	969	25.710	27.429	19.810	1.00 29.20
ATOM	1090	C	ASN	B	969	25.291	28.803	20.297	1.00 30.35
ATOM	1091	O	ASN	B	969	24.086	29.145	20.204	1.00 30.32
ATOM	1092	CB	ASN	B	969	24.598	26.375	20.098	1.00 25.04
ATOM	1093	CG	ASN	B	969	24.914	25.020	19.495	1.00 30.26
ATOM	1094	OD1	ASN	B	969	25.378	24.869	18.361	1.00 32.57
ATOM	1095	ND2	ASN	B	969	24.648	23.886	20.172	1.00 28.51
ATOM	1096	N	ILE	B	970	26.257	29.496	20.910	1.00 27.55
ATOM	1097	CA	ILE	B	970	26.015	30.841	21.418	1.00 28.82
ATOM	1098	C	ILE	B	970	26.802	31.795	20.505	1.00 29.55
ATOM	1099	O	ILE	B	970	27.963	31.487	20.196	1.00 27.59
ATOM	1100	CB	ILE	B	970	26.412	31.038	22.895	1.00 26.22
ATOM	1101	CG1	ILE	B	970	25.618	30.198	23.893	1.00 25.70
ATOM	1102	CG2	ILE	B	970	26.312	32.536	23.261	1.00 21.48
ATOM	1103	CD1	ILE	B	970	24.088	30.263	23.734	1.00 23.69
ATOM	1104	N	LEU	B	971	26.208	32.904	20.028	1.00 29.96
ATOM	1105	CA	LEU	B	971	26.961	33.826	19.172	1.00 30.19
ATOM	1106	C	LEU	B	971	27.438	35.090	19.845	1.00 31.70
ATOM	1107	O	LEU	B	971	26.784	35.584	20.761	1.00 33.46
ATOM	1108	CB	LEU	B	971	26.085	34.128	17.930	1.00 30.67
ATOM	1109	CG	LEU	B	971	25.855	32.975	16.964	1.00 34.15
ATOM	1110	CD1	LEU	B	971	24.695	33.281	15.982	1.00 33.06
ATOM	1111	CD2	LEU	B	971	27.122	32.553	16.185	1.00 30.70
ATOM	1112	N	VAL	B	972	28.541	35.731	19.447	1.00 30.83
ATOM	1113	CA	VAL	B	972	29.044	36.982	20.037	1.00 32.48
ATOM	1114	C	VAL	B	972	28.758	38.104	19.005	1.00 30.36
ATOM	1115	O	VAL	B	972	29.405	38.186	17.951	1.00 31.08
ATOM	1116	CB	VAL	B	972	30.521	36.984	20.420	1.00 32.58
ATOM	1117	CG1	VAL	B	972	30.930	38.281	21.136	1.00 34.22
ATOM	1118	CG2	VAL	B	972	30.871	35.785	21.333	1.00 31.21
ATOM	1119	N	GLY	B	973	27.711	38.847	19.310	1.00 30.33
ATOM	1120	CA	GLY	B	973	27.207	39.802	18.315	1.00 29.88
ATOM	1121	C	GLY	B	973	27.727	41.204	18.479	1.00 32.70
ATOM	1122	O	GLY	B	973	28.585	41.451	19.329	1.00 31.01
ATOM	1123	N	GLU	B	974	27.145	42.135	17.747	1.00 34.65
ATOM	1124	CA	GLU	B	974	27.522	43.527	17.855	1.00 33.72
ATOM	1125	C	GLU	B	974	27.649	43.930	19.302	1.00 33.97
ATOM	1126	O	GLU	B	974	26.870	43.530	20.180	1.00 30.31
ATOM	1127	CB	GLU	B	974	26.420	44.367	17.187	1.00 40.43
ATOM	1128	CG	GLU	B	974	26.557	44.283	15.649	1.00 48.26
ATOM	1129	CD	GLU	B	974	26.317	45.679	15.071	1.00 54.12
ATOM	1130	OE1	GLU	B	974	25.119	46.052	15.074	1.00 56.77
ATOM	1131	OE2	GLU	B	974	27.258	46.414	14.674	1.00 56.47
ATOM	1132	N	ASN	B	975	28.679	44.730	19.612	1.00 32.99
ATOM	1133	CA	ASN	B	975	28.909	45.235	20.945	1.00 32.09
ATOM	1134	C	ASN	B	975	29.202	44.081	21.877	1.00 32.69
ATOM	1135	O	ASN	B	975	29.082	44.240	23.098	1.00 33.59

FIG. 5T

ATOM	1136	CB	ASN	B	975	27.642	46.019	21.385	1.00	36.61
ATOM	1137	CG	ASN	B	975	27.446	47.285	20.540	1.00	37.11
ATOM	1138	OD1	ASN	B	975	26.276	47.739	20.363	1.00	39.26
ATOM	1139	ND2	ASN	B	975	28.530	47.826	20.042	1.00	29.86
ATOM	1140	N	TYR	B	976	29.715	42.945	21.379	1.00	32.96
ATOM	1141	CA	TYR	B	976	29.974	41.815	22.291	1.00	33.87
ATOM	1142	C	TYR	B	976	28.745	41.291	22.977	1.00	33.96
ATOM	1143	O	TYR	B	976	28.952	40.845	24.142	1.00	38.50
ATOM	1144	CB	TYR	B	976	31.090	42.145	23.319	1.00	32.57
ATOM	1145	CG	TYR	B	976	32.316	42.635	22.562	1.00	34.93
ATOM	1146	CD1	TYR	B	976	32.643	43.977	22.488	1.00	34.96
ATOM	1147	CD2	TYR	B	976	33.064	41.750	21.796	1.00	36.25
ATOM	1148	CE1	TYR	B	976	33.734	44.404	21.765	1.00	36.57
ATOM	1149	CE2	TYR	B	976	34.151	42.185	21.066	1.00	37.74
ATOM	1150	CZ	TYR	B	976	34.469	43.524	21.027	1.00	38.58
ATOM	1151	OH	TYR	B	976	35.544	43.988	20.318	1.00	41.08
ATOM	1152	N	VAL	B	977	27.498	41.318	22.583	1.00	33.38
ATOM	1153	CA	VAL	B	977	26.363	40.804	23.354	1.00	30.29
ATOM	1154	C	VAL	B	977	26.160	39.324	23.034	1.00	28.06
ATOM	1155	O	VAL	B	977	26.157	38.975	21.853	1.00	30.23
ATOM	1156	CB	VAL	B	977	25.135	41.674	23.014	1.00	29.39
ATOM	1157	CG1	VAL	B	977	23.846	41.027	23.499	1.00	28.20
ATOM	1158	CG2	VAL	B	977	25.284	43.038	23.718	1.00	31.72
ATOM	1159	N	ALA	B	978	26.159	38.459	24.028	1.00	27.76
ATOM	1160	CA	ALA	B	978	25.975	37.006	23.681	1.00	28.79
ATOM	1161	C	ALA	B	978	24.563	36.847	23.132	1.00	31.90
ATOM	1162	O	ALA	B	978	23.647	37.514	23.577	1.00	30.56
ATOM	1163	CB	ALA	B	978	26.186	36.192	24.917	1.00	25.90
ATOM	1164	N	LYS	B	979	24.330	36.043	22.103	1.00	33.62
ATOM	1165	CA	LYS	B	979	23.070	35.784	21.463	1.00	31.66
ATOM	1166	C	LYS	B	979	22.780	34.287	21.336	1.00	31.79
ATOM	1167	O	LYS	B	979	23.561	33.490	20.808	1.00	29.59
ATOM	1168	CB	LYS	B	979	23.102	36.390	20.030	1.00	34.05
ATOM	1169	CG	LYS	B	979	22.883	37.917	20.237	1.00	38.30
ATOM	1170	CD	LYS	B	979	23.149	38.766	19.049	1.00	36.22
ATOM	1171	CE	LYS	B	979	23.157	40.252	19.366	1.00	39.70
ATOM	1172	NZ	LYS	B	979	21.788	40.833	19.313	1.00	39.24
ATOM	1173	N	ILE	B	980	21.643	33.866	21.839	1.00	29.92
ATOM	1174	CA	ILE	B	980	21.279	32.444	21.718	1.00	29.31
ATOM	1175	C	ILE	B	980	20.877	32.083	20.290	1.00	32.94
ATOM	1176	O	ILE	B	980	20.093	32.771	19.620	1.00	34.86
ATOM	1177	CB	ILE	B	980	20.142	32.123	22.676	1.00	27.87
ATOM	1178	CG1	ILE	B	980	20.564	32.314	24.120	1.00	29.18
ATOM	1179	CG2	ILE	B	980	19.778	30.614	22.519	1.00	32.98
ATOM	1180	CD1	ILE	B	980	19.477	32.141	25.157	1.00	26.99
ATOM	1181	N	ALA	B	981	21.425	30.940	19.843	1.00	33.63
ATOM	1182	CA	ALA	B	981	21.100	30.397	18.542	1.00	34.72
ATOM	1183	C	ALA	B	981	20.872	28.883	18.597	1.00	36.94
ATOM	1184	O	ALA	B	981	20.993	28.205	19.630	1.00	36.37
ATOM	1185	CB	ALA	B	981	22.158	30.764	17.532	1.00	32.74
ATOM	1186	N	ASP	B	982	20.702	28.316	17.416	1.00	38.89
ATOM	1187	CA	ASP	B	982	20.540	26.898	17.122	1.00	38.46
ATOM	1188	C	ASP	B	982	19.195	26.448	17.713	1.00	37.99
ATOM	1189	O	ASP	B	982	19.092	25.674	18.675	1.00	36.61
ATOM	1190	CB	ASP	B	982	21.703	26.016	17.541	1.00	40.25
ATOM	1191	CG	ASP	B	982	21.452	24.552	17.184	1.00	43.41
ATOM	1192	OD1	ASP	B	982	20.728	24.230	16.205	1.00	46.24

FIG. 5U

ATOM	1193	OD2	ASP	B	982	21.281	23.629	17.877	1.00	42.63
ATOM	1194	N	PHE	B	983	18.165	27.008	17.126	1.00	36.77
ATOM	1195	CA	PHE	B	983	16.782	26.774	17.503	1.00	41.16
ATOM	1196	C	PHE	B	983	16.065	25.567	16.890	1.00	42.48
ATOM	1197	O	PHE	B	983	16.087	25.257	15.684	1.00	43.89
ATOM	1198	CB	PHE	B	983	15.964	28.059	17.163	1.00	39.87
ATOM	1199	CG	PHE	B	983	16.280	29.135	18.179	1.00	39.48
ATOM	1200	CD1	PHE	B	983	15.940	28.923	19.504	1.00	38.68
ATOM	1201	CD2	PHE	B	983	16.957	30.289	17.825	1.00	39.97
ATOM	1202	CE1	PHE	B	983	16.251	29.809	20.491	1.00	37.05
ATOM	1203	CE2	PHE	B	983	17.257	31.221	18.816	1.00	40.42
ATOM	1204	CZ	PHE	B	983	16.906	30.993	20.135	1.00	39.41
ATOM	1205	N	GLY	B	984	15.346	24.852	17.733	1.00	41.51
ATOM	1206	CA	GLY	B	984	14.461	23.724	17.265	1.00	41.21
ATOM	1207	C	GLY	B	984	13.535	23.685	18.500	1.00	40.75
ATOM	1208	O	GLY	B	984	13.678	22.812	19.368	1.00	40.87
ATOM	1209	N	LEU	B	985	12.781	24.779	18.612	1.00	38.40
ATOM	1210	CA	LEU	B	985	12.020	25.010	19.826	1.00	38.54
ATOM	1211	C	LEU	B	985	10.844	24.053	20.021	1.00	39.23
ATOM	1212	O	LEU	B	985	10.331	23.451	19.099	1.00	39.81
ATOM	1213	CB	LEU	B	985	11.597	26.477	19.879	1.00	38.29
ATOM	1214	CG	LEU	B	985	12.703	27.505	20.071	1.00	39.62
ATOM	1215	CD1	LEU	B	985	12.112	28.913	19.963	1.00	41.67
ATOM	1216	CD2	LEU	B	985	13.378	27.375	21.450	1.00	40.64
ATOM	1217	N	SER	B	986	10.420	23.923	21.268	1.00	38.75
ATOM	1218	CA	SER	B	986	9.258	23.124	21.640	1.00	41.57
ATOM	1219	C	SER	B	986	8.618	23.946	22.764	1.00	41.04
ATOM	1220	O	SER	B	986	9.376	24.681	23.389	1.00	40.97
ATOM	1221	CB	SER	B	986	9.623	21.781	22.276	1.00	41.12
ATOM	1222	OG	SER	B	986	10.132	20.965	21.268	1.00	44.70
ATOM	1223	N	ARG	B	987	7.306	23.872	22.881	1.00	41.47
ATOM	1224	CA	ARG	B	987	6.579	24.634	23.849	1.00	39.96
ATOM	1225	C	ARG	B	987	5.664	23.672	24.592	1.00	39.46
ATOM	1226	O	ARG	B	987	4.928	22.897	24.001	1.00	40.85
ATOM	1227	CB	ARG	B	987	5.759	25.671	23.100	1.00	42.69
ATOM	1228	CG	ARG	B	987	5.518	26.881	23.980	1.00	43.46
ATOM	1229	CD	ARG	B	987	4.820	27.932	23.102	1.00	47.12
ATOM	1230	NE	ARG	B	987	4.503	29.062	23.969	1.00	48.45
ATOM	1231	CZ	ARG	B	987	4.042	30.245	23.498	1.00	49.30
ATOM	1232	NH1	ARG	B	987	3.859	30.446	22.195	1.00	47.75
ATOM	1233	NH2	ARG	B	987	3.820	31.126	24.461	1.00	47.10
ATOM	1234	N	GLY	B	988	5.803	23.678	25.895	1.00	36.84
ATOM	1235	CA	GLY	B	988	5.310	22.780	26.860	1.00	37.53
ATOM	1236	C	GLY	B	988	6.133	22.613	28.131	1.00	39.84
ATOM	1237	O	GLY	B	988	7.113	23.319	28.413	1.00	37.68
ATOM	1238	N	GLN	B	989	5.621	21.679	28.931	1.00	37.98
ATOM	1239	CA	GLN	B	989	6.211	21.351	30.208	1.00	36.52
ATOM	1240	C	GLN	B	989	7.342	20.344	29.982	1.00	36.26
ATOM	1241	O	GLN	B	989	8.364	20.451	30.678	1.00	35.23
ATOM	1242	CB	GLN	B	989	5.134	20.856	31.154	1.00	36.36
ATOM	1243	CG	GLN	B	989	5.676	20.186	32.391	1.00	39.62
ATOM	1244	CD	GLN	B	989	4.653	19.836	33.425	1.00	39.25
ATOM	1245	OE1	GLN	B	989	4.232	20.788	34.082	1.00	42.73
ATOM	1246	NE2	GLN	B	989	4.255	18.604	33.639	1.00	40.97
ATOM	1247	N	GLU	B	990	7.214	19.459	28.997	1.00	33.95
ATOM	1248	CA	GLU	B	990	8.362	18.545	28.745	1.00	32.76
ATOM	1249	C	GLU	B	990	8.318	18.162	27.281	1.00	31.62

FIG. 5V

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ATOM   1250  O   GLU B 990       7.134  18.267  26.782  1.00 35.90
ATOM   1251  CB  GLU B 990       8.324  17.321  29.615  1.00 32.06
ATOM   1252  CG  GLU B 990       7.034  16.491  29.549  1.00 34.29
ATOM   1253  CD  GLU B 990       5.855  16.986  30.361  1.00 35.18
ATOM   1254  OE1 GLU B 990       4.741  17.354  29.866  1.00 31.61
ATOM   1255  OE2 GLU B 990       5.907  17.055  31.606  1.00 37.46
ATOM   1256  N   VAL B 991       9.245  17.586  26.636  1.00 28.59
ATOM   1257  CA  VAL B 991       9.254  17.187  25.250  1.00 27.10
ATOM   1258  C   VAL B 991      10.294  16.035  25.123  1.00 34.31
ATOM   1259  O   VAL B 991      11.499  16.047  25.461  1.00 34.01
ATOM   1260  CB  VAL B 991       9.566  18.341  24.297  1.00 27.78
ATOM   1261  CG1 VAL B 991      10.981  18.939  24.577  1.00 28.52
ATOM   1262  CG2 VAL B 991       9.531  17.878  22.827  1.00 26.55
ATOM   1263  N   TYR B 992       9.815  15.116  24.284  1.00 33.22
ATOM   1264  CA  TYR B 992      10.510  13.950  23.872  1.00 35.07
ATOM   1265  C   TYR B 992      11.168  14.196  22.521  1.00 36.09
ATOM   1266  O   TYR B 992      10.453  14.723  21.653  1.00 37.35
ATOM   1267  CB  TYR B 992       9.504  12.750  23.851  1.00 32.12
ATOM   1268  CG  TYR B 992      10.187  11.588  23.154  1.00 34.00
ATOM   1269  CD1 TYR B 992      10.952  10.664  23.855  1.00 35.23
ATOM   1270  CD2 TYR B 992      10.065  11.491  21.767  1.00 34.41
ATOM   1271  CE1 TYR B 992      11.597   9.629  23.205  1.00 34.80
ATOM   1272  CE2 TYR B 992      10.706  10.464  21.115  1.00 35.88
ATOM   1273  CZ  TYR B 992      11.471   9.575  21.830  1.00 37.31
ATOM   1274  OH  TYR B 992      12.090   8.582  21.090  1.00 41.58
ATOM   1275  N   VAL B 993      12.465  13.922  22.409  1.00 35.09
ATOM   1276  CA  VAL B 993      13.166  14.093  21.148  1.00 40.55
ATOM   1277  C   VAL B 993      14.192  12.937  21.077  1.00 44.20
ATOM   1278  O   VAL B 993      14.924  12.698  22.027  1.00 41.10
ATOM   1279  CB  VAL B 993      14.027  15.345  20.884  1.00 40.80
ATOM   1280  CG1 VAL B 993      14.377  15.434  19.397  1.00 41.00
ATOM   1281  CG2 VAL B 993      13.444  16.675  21.308  1.00 40.65
ATOM   1282  N   LYS B 994      14.248  12.280  19.929  1.00 52.91
ATOM   1283  CA  LYS B 994      15.228  11.218  19.681  1.00 59.67
ATOM   1284  C   LYS B 994      16.314  11.668  18.722  1.00 63.50
ATOM   1285  O   LYS B 994      15.968  12.346  17.752  1.00 65.43
ATOM   1286  CB  LYS B 994      14.452  10.051  19.050  1.00 62.12
ATOM   1287  CG  LYS B 994      15.258   9.165  18.114  1.00 64.47
ATOM   1288  CD  LYS B 994      14.523   7.917  17.676  1.00 66.81
ATOM   1289  CE  LYS B 994      14.741   6.737  18.627  1.00 69.22
ATOM   1290  NZ  LYS B 994      16.113   6.131  18.446  1.00 70.28
ATOM   1291  N   LYS B 995      17.568  11.244  18.841  1.00 68.11
ATOM   1292  CA  LYS B 995      18.698  11.497  17.964  1.00 69.33
ATOM   1293  C   LYS B 995      19.277  12.900  17.869  1.00 71.04
ATOM   1294  CB  LYS B 995      18.387  11.058  16.520  1.00 68.75
ATOM   1295  N   THR B 996      19.210  13.731  18.891  1.00 72.92
ATOM   1296  CA  THR B 996      19.849  15.039  18.958  1.00 74.27
ATOM   1297  C   THR B 996      18.897  16.170  18.571  1.00 74.88
ATOM   1298  O   THR B 996      17.742  15.867  18.197  1.00 75.62
ATOM   1299  CB  THR B 996      21.108  15.075  18.098  1.00 74.16
TER
ATOM   1300  N   LEU C1000     24.923  13.250  19.201  1.00 61.56
ATOM   1301  CA  LEU C1000     24.606  13.627  20.610  1.00 60.45
ATOM   1302  C   LEU C1000     25.273  14.888  21.132  1.00 59.31
ATOM   1303  O   LEU C1000     25.926  15.737  20.498  1.00 61.19
ATOM   1304  CB  LEU C1000     25.085  12.439  21.459  1.00 62.33
ATOM   1305  N   PRO C1001     25.106  15.086  22.450  1.00 55.81
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FIG. 5W

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ATOM   1306  CA  PRO C1001      25.717  16.238  23.154  1.00 47.68
ATOM   1307  C   PRO C1001      25.633  15.865  24.622  1.00 42.57
ATOM   1308  O   PRO C1001      25.066  16.507  25.497  1.00 42.56
ATOM   1309  CB  PRO C1001      25.055  17.514  22.761  1.00 49.13
ATOM   1310  N   VAL C1002      26.137  14.628  24.881  1.00 39.19
ATOM   1311  CA  VAL C1002      26.105  13.982  26.180  1.00 36.21
ATOM   1312  C   VAL C1002      26.526  14.731  27.414  1.00 32.43
ATOM   1313  O   VAL C1002      25.981  14.707  28.510  1.00 29.30
ATOM   1314  CB  VAL C1002      27.129  12.774  26.075  1.00 38.41
ATOM   1315  CG1 VAL C1002      27.304  12.077  27.400  1.00 36.91
ATOM   1316  CG2 VAL C1002      26.315  11.872  25.131  1.00 39.50
ATOM   1317  N   ARG C1003      27.699  15.354  27.317  1.00 35.49
ATOM   1318  CA  ARG C1003      28.454  16.101  28.310  1.00 34.85
ATOM   1319  C   ARG C1003      27.745  17.378  28.731  1.00 32.80
ATOM   1320  O   ARG C1003      28.073  18.089  29.675  1.00 33.09
ATOM   1321  CB  ARG C1003      29.877  16.407  27.775  1.00 35.57
ATOM   1322  CG  ARG C1003      30.017  15.726  26.418  1.00 40.79
ATOM   1323  CD  ARG C1003      31.524  15.638  26.082  1.00 42.74
ATOM   1324  NE  ARG C1003      32.199  15.018  27.219  1.00 46.61
ATOM   1325  CZ  ARG C1003      33.482  14.536  26.897  1.00 42.40
ATOM   1326  NH1 ARG C1003      33.675  14.646  25.606  1.00 44.69
ATOM   1327  NH2 ARG C1003      34.058  13.991  27.899  1.00 41.82
ATOM   1328  N   TRP C1004      26.753  17.765  27.983  1.00 31.57
ATOM   1329  CA  TRP C1004      25.743  18.792  28.171  1.00 32.26
ATOM   1330  C   TRP C1004      24.352  18.357  28.588  1.00 33.31
ATOM   1331  O   TRP C1004      23.571  19.223  29.047  1.00 32.82
ATOM   1332  CB  TRP C1004      25.513  19.633  26.877  1.00 31.61
ATOM   1333  CG  TRP C1004      26.794  20.424  26.649  1.00 29.75
ATOM   1334  CD1 TRP C1004      27.065  21.659  27.174  1.00 33.83
ATOM   1335  CD2 TRP C1004      27.885  20.016  25.845  1.00 30.53
ATOM   1336  NE1 TRP C1004      28.350  22.036  26.758  1.00 30.12
ATOM   1337  CE2 TRP C1004      28.838  21.058  25.939  1.00 32.87
ATOM   1338  CE3 TRP C1004      28.284  18.907  25.081  1.00 31.33
ATOM   1339  CZ2 TRP C1004      30.114  21.052  25.322  1.00 31.29
ATOM   1340  CZ3 TRP C1004      29.523  18.911  24.457  1.00 31.61
ATOM   1341  CH2 TRP C1004      30.442  19.974  24.537  1.00 31.26
ATOM   1342  N   MET C1005      24.039  17.058  28.523  1.00 31.05
ATOM   1343  CA  MET C1005      22.691  16.644  28.871  1.00 30.92
ATOM   1344  C   MET C1005      22.482  16.372  30.342  1.00 31.46
ATOM   1345  O   MET C1005      23.344  15.779  30.955  1.00 30.88
ATOM   1346  CB  MET C1005      22.425  15.401  28.027  1.00 35.15
ATOM   1347  CG  MET C1005      22.250  15.671  26.542  1.00 35.78
ATOM   1348  SD  MET C1005      22.331  14.145  25.574  1.00 43.66
ATOM   1349  CE  MET C1005      20.582  13.671  25.658  1.00 39.42
ATOM   1350  N   ALA C1006      21.331  16.767  30.898  1.00 30.39
ATOM   1351  CA  ALA C1006      20.980  16.384  32.257  1.00 32.23
ATOM   1352  C   ALA C1006      20.903  14.819  32.255  1.00 29.50
ATOM   1353  O   ALA C1006      20.820  14.243  31.191  1.00 25.95
ATOM   1354  CB  ALA C1006      19.558  16.827  32.686  1.00 32.19
ATOM   1355  N   ILE C1007      21.063  14.271  33.415  1.00 28.66
ATOM   1356  CA  ILE C1007      20.991  12.831  33.717  1.00 34.31
ATOM   1357  C   ILE C1007      19.626  12.254  33.361  1.00 32.33
ATOM   1358  O   ILE C1007      19.539  11.314  32.569  1.00 34.27
ATOM   1359  CB  ILE C1007      21.316  12.831  35.238  1.00 36.74
ATOM   1360  CG1 ILE C1007      22.831  12.539  35.418  1.00 40.16
ATOM   1361  CG2 ILE C1007      20.535  11.850  36.027  1.00 41.55
ATOM   1362  CD1 ILE C1007      23.298  12.738  36.843  1.00 39.53
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FIG. 5X

ATOM	1363	N	GLU	C1008	18.515	12.879	33.668	1.00	32.21
ATOM	1364	CA	GLU	C1008	17.179	12.414	33.238	1.00	30.51
ATOM	1365	C	GLU	C1008	17.097	12.390	31.725	1.00	30.14
ATOM	1366	O	GLU	C1008	16.588	11.399	31.127	1.00	30.02
ATOM	1367	CB	GLU	C1008	16.079	13.201	33.887	1.00	32.29
ATOM	1368	CG	GLU	C1008	15.861	14.623	33.271	1.00	31.03
ATOM	1369	CD	GLU	C1008	16.672	15.611	34.070	1.00	30.62
ATOM	1370	OE1	GLU	C1008	17.610	15.181	34.800	1.00	33.04
ATOM	1371	OE2	GLU	C1008	16.405	16.824	34.011	1.00	33.30
ATOM	1372	N	SER	C1009	17.652	13.397	31.054	1.00	28.64
ATOM	1373	CA	SER	C1009	17.665	13.395	29.574	1.00	27.96
ATOM	1374	C	SER	C1009	18.581	12.320	29.008	1.00	32.36
ATOM	1375	O	SER	C1009	18.258	11.867	27.889	1.00	33.49
ATOM	1376	CB	SER	C1009	18.120	14.740	29.001	1.00	27.04
ATOM	1377	OG	SER	C1009	17.266	15.856	29.232	1.00	29.52
ATOM	1378	N	LEU	C1010	19.732	11.948	29.646	1.00	30.58
ATOM	1379	CA	LEU	C1010	20.458	10.834	29.043	1.00	33.82
ATOM	1380	C	LEU	C1010	19.587	9.543	29.184	1.00	34.58
ATOM	1381	O	LEU	C1010	19.600	8.647	28.340	1.00	33.77
ATOM	1382	CB	LEU	C1010	21.835	10.478	29.678	1.00	34.39
ATOM	1383	CG	LEU	C1010	22.839	11.659	29.618	1.00	34.04
ATOM	1384	CD1	LEU	C1010	23.989	11.636	30.582	1.00	35.06
ATOM	1385	CD2	LEU	C1010	23.324	11.698	28.183	1.00	34.32
ATOM	1386	N	ASN	C1011	18.894	9.423	30.317	1.00	34.50
ATOM	1387	CA	ASN	C1011	18.175	8.188	30.585	1.00	39.53
ATOM	1388	C	ASN	C1011	16.867	8.049	29.814	1.00	39.46
ATOM	1389	O	ASN	C1011	16.521	6.887	29.507	1.00	41.72
ATOM	1390	CB	ASN	C1011	17.744	7.990	32.055	1.00	37.12
ATOM	1391	CG	ASN	C1011	18.994	7.594	32.849	1.00	40.42
ATOM	1392	OD1	ASN	C1011	19.913	7.055	32.211	1.00	41.43
ATOM	1393	ND2	ASN	C1011	18.990	7.876	34.135	1.00	37.03
ATOM	1394	N	TYR	C1012	16.144	9.174	29.765	1.00	36.32
ATOM	1395	CA	TYR	C1012	14.765	9.067	29.205	1.00	33.71
ATOM	1396	C	TYR	C1012	14.644	9.864	27.929	1.00	37.07
ATOM	1397	O	TYR	C1012	13.431	9.936	27.557	1.00	39.06
ATOM	1398	CB	TYR	C1012	13.779	9.722	30.189	1.00	25.11
ATOM	1399	CG	TYR	C1012	13.979	9.247	31.601	1.00	26.79
ATOM	1400	CD1	TYR	C1012	13.915	10.061	32.704	1.00	28.02
ATOM	1401	CD2	TYR	C1012	14.199	7.868	31.824	1.00	29.96
ATOM	1402	CE1	TYR	C1012	14.075	9.560	33.984	1.00	31.07
ATOM	1403	CE2	TYR	C1012	14.378	7.325	33.070	1.00	30.68
ATOM	1404	CZ	TYR	C1012	14.310	8.194	34.126	1.00	32.85
ATOM	1405	OH	TYR	C1012	14.494	7.677	35.423	1.00	38.60
ATOM	1406	N	SER	C1013	15.568	10.695	27.480	1.00	35.61
ATOM	1407	CA	SER	C1013	15.244	11.547	26.340	1.00	36.12
ATOM	1408	C	SER	C1013	14.080	12.522	26.555	1.00	31.92
ATOM	1409	O	SER	C1013	13.533	12.997	25.558	1.00	29.49
ATOM	1410	CB	SER	C1013	15.021	10.764	25.075	1.00	38.37
ATOM	1411	OG	SER	C1013	16.000	9.929	24.605	1.00	39.85
ATOM	1412	N	VAL	C1014	13.848	12.926	27.798	1.00	34.71
ATOM	1413	CA	VAL	C1014	12.887	13.999	28.005	1.00	34.17
ATOM	1414	C	VAL	C1014	13.761	15.212	28.406	1.00	32.14
ATOM	1415	O	VAL	C1014	14.764	15.102	29.061	1.00	31.92
ATOM	1416	CB	VAL	C1014	11.803	13.647	29.007	1.00	35.91
ATOM	1417	CG1	VAL	C1014	10.773	14.771	28.958	1.00	35.03
ATOM	1418	CG2	VAL	C1014	11.129	12.316	28.672	1.00	35.03
ATOM	1419	N	TYR	C1015	13.255	16.377	27.994	1.00	33.31

FIG. 5Y

ATOM	1420	CA	TYR	C1015	13.917	17.662	28.232	1.00	29.96
ATOM	1421	C	TYR	C1015	12.870	18.627	28.713	1.00	32.82
ATOM	1422	O	TYR	C1015	11.635	18.497	28.361	1.00	33.09
ATOM	1423	CB	TYR	C1015	14.268	18.208	26.817	1.00	31.34
ATOM	1424	CG	TYR	C1015	15.273	17.339	26.106	1.00	32.85
ATOM	1425	CD1	TYR	C1015	14.953	16.293	25.270	1.00	33.14
ATOM	1426	CD2	TYR	C1015	16.625	17.556	26.338	1.00	33.80
ATOM	1427	CE1	TYR	C1015	15.892	15.497	24.664	1.00	36.71
ATOM	1428	CE2	TYR	C1015	17.623	16.791	25.745	1.00	36.63
ATOM	1429	CZ	TYR	C1015	17.249	15.758	24.895	1.00	36.99
ATOM	1430	OH	TYR	C1015	18.233	15.005	24.325	1.00	37.59
ATOM	1431	N	THR	C1016	13.210	19.409	29.691	1.00	29.91
ATOM	1432	CA	THR	C1016	12.342	20.393	30.312	1.00	30.08
ATOM	1433	C	THR	C1016	13.109	21.700	30.459	1.00	33.68
ATOM	1434	O	THR	C1016	14.307	21.752	30.085	1.00	32.46
ATOM	1435	CB	THR	C1016	11.986	19.882	31.717	1.00	31.45
ATOM	1436	OG1	THR	C1016	13.149	19.778	32.540	1.00	31.21
ATOM	1437	CG2	THR	C1016	11.332	18.415	31.720	1.00	29.42
ATOM	1438	N	THR	C1017	12.509	22.699	31.141	1.00	31.49
ATOM	1439	CA	THR	C1017	13.301	23.863	31.536	1.00	32.10
ATOM	1440	C	THR	C1017	14.367	23.447	32.536	1.00	33.86
ATOM	1441	O	THR	C1017	15.480	24.004	32.588	1.00	31.99
ATOM	1442	CB	THR	C1017	12.396	25.033	32.078	1.00	32.15
ATOM	1443	OG1	THR	C1017	11.836	25.456	30.829	1.00	32.91
ATOM	1444	CG2	THR	C1017	13.152	26.192	32.675	1.00	30.94
ATOM	1445	N	ASN	C1018	14.062	22.468	33.403	1.00	32.36
ATOM	1446	CA	ASN	C1018	15.020	21.997	34.372	1.00	34.23
ATOM	1447	C	ASN	C1018	16.208	21.329	33.647	1.00	33.65
ATOM	1448	O	ASN	C1018	17.326	21.560	34.163	1.00	32.63
ATOM	1449	CB	ASN	C1018	14.563	21.089	35.519	1.00	33.92
ATOM	1450	CG	ASN	C1018	13.478	21.750	36.390	1.00	36.18
ATOM	1451	OD1	ASN	C1018	13.561	22.943	36.772	1.00	33.93
ATOM	1452	ND2	ASN	C1018	12.400	20.983	36.687	1.00	31.82
ATOM	1453	N	SER	C1019	16.007	20.738	32.468	1.00	30.11
ATOM	1454	CA	SER	C1019	17.216	20.101	31.865	1.00	31.68
ATOM	1455	C	SER	C1019	18.016	21.121	31.069	1.00	30.62
ATOM	1456	O	SER	C1019	19.237	21.110	30.787	1.00	25.61
ATOM	1457	CB	SER	C1019	16.668	18.883	31.150	1.00	29.04
ATOM	1458	OG	SER	C1019	16.208	19.177	29.829	1.00	30.35
ATOM	1459	N	ASP	C1020	17.331	22.228	30.738	1.00	30.23
ATOM	1460	CA	ASP	C1020	17.923	23.429	30.164	1.00	27.36
ATOM	1461	C	ASP	C1020	18.880	24.034	31.183	1.00	26.47
ATOM	1462	O	ASP	C1020	19.935	24.477	30.766	1.00	28.27
ATOM	1463	CB	ASP	C1020	16.986	24.536	29.714	1.00	28.00
ATOM	1464	CG	ASP	C1020	16.480	24.298	28.328	1.00	28.71
ATOM	1465	OD1	ASP	C1020	16.969	23.343	27.647	1.00	31.13
ATOM	1466	OD2	ASP	C1020	15.583	24.984	27.876	1.00	32.14
ATOM	1467	N	VAL	C1021	18.502	24.085	32.455	1.00	26.65
ATOM	1468	CA	VAL	C1021	19.328	24.627	33.497	1.00	26.02
ATOM	1469	C	VAL	C1021	20.546	23.742	33.781	1.00	27.12
ATOM	1470	O	VAL	C1021	21.575	24.333	34.098	1.00	23.97
ATOM	1471	CB	VAL	C1021	18.525	24.925	34.779	1.00	27.32
ATOM	1472	CG1	VAL	C1021	19.464	25.263	35.929	1.00	25.33
ATOM	1473	CG2	VAL	C1021	17.590	26.138	34.626	1.00	29.37
ATOM	1474	N	TRP	C1022	20.461	22.409	33.671	1.00	25.32
ATOM	1475	CA	TRP	C1022	21.679	21.587	33.868	1.00	23.28
ATOM	1476	C	TRP	C1022	22.664	21.958	32.796	1.00	23.00

FIG. 5Z

ATOM	1477	O	TRP	C1022	23.835	22.338	32.917	1.00	25.36
ATOM	1478	CB	TRP	C1022	21.248	20.096	33.625	1.00	25.77
ATOM	1479	CG	TRP	C1022	22.434	19.150	33.646	1.00	27.35
ATOM	1480	CD1	TRP	C1022	23.411	18.987	32.695	1.00	26.63
ATOM	1481	CD2	TRP	C1022	22.685	18.200	34.675	1.00	28.39
ATOM	1482	NE1	TRP	C1022	24.267	18.008	33.079	1.00	29.90
ATOM	1483	CE2	TRP	C1022	23.840	17.481	34.300	1.00	30.24
ATOM	1484	CE3	TRP	C1022	22.041	17.867	35.866	1.00	30.30
ATOM	1485	CZ2	TRP	C1022	24.394	16.485	35.090	1.00	32.33
ATOM	1486	CZ3	TRP	C1022	22.563	16.816	36.624	1.00	31.39
ATOM	1487	CH2	TRP	C1022	23.718	16.151	36.243	1.00	32.10
ATOM	1488	N	SER	C1023	22.207	21.928	31.529	1.00	21.23
ATOM	1489	CA	SER	C1023	23.068	22.354	30.379	1.00	22.80
ATOM	1490	C	SER	C1023	23.618	23.745	30.495	1.00	27.97
ATOM	1491	O	SER	C1023	24.829	24.031	30.146	1.00	23.26
ATOM	1492	CB	SER	C1023	22.108	21.769	29.326	1.00	24.28
ATOM	1493	OG	SER	C1023	21.977	22.454	28.131	1.00	34.21
ATOM	1494	N	TYR	C1024	22.810	24.769	30.968	1.00	24.68
ATOM	1495	CA	TYR	C1024	23.395	26.101	31.223	1.00	25.91
ATOM	1496	C	TYR	C1024	24.614	26.083	32.155	1.00	28.55
ATOM	1497	O	TYR	C1024	25.582	26.856	32.091	1.00	26.16
ATOM	1498	CB	TYR	C1024	22.317	27.041	31.808	1.00	23.53
ATOM	1499	CG	TYR	C1024	22.904	28.385	32.225	1.00	23.34
ATOM	1500	CD1	TYR	C1024	22.931	29.409	31.328	1.00	21.89
ATOM	1501	CD2	TYR	C1024	23.322	28.564	33.537	1.00	21.62
ATOM	1502	CE1	TYR	C1024	23.498	30.640	31.655	1.00	24.95
ATOM	1503	CE2	TYR	C1024	23.929	29.791	33.858	1.00	25.56
ATOM	1504	CZ	TYR	C1024	23.957	30.795	32.941	1.00	24.77
ATOM	1505	OH	TYR	C1024	24.513	32.006	33.282	1.00	29.84
ATOM	1506	N	GLY	C1025	24.559	25.263	33.180	1.00	31.16
ATOM	1507	CA	GLY	C1025	25.499	24.901	34.180	1.00	28.63
ATOM	1508	C	GLY	C1025	26.812	24.444	33.475	1.00	29.18
ATOM	1509	O	GLY	C1025	27.826	24.973	33.911	1.00	25.38
ATOM	1510	N	VAL	C1026	26.724	23.628	32.431	1.00	30.48
ATOM	1511	CA	VAL	C1026	27.848	23.171	31.665	1.00	30.49
ATOM	1512	C	VAL	C1026	28.404	24.335	30.867	1.00	30.61
ATOM	1513	O	VAL	C1026	29.622	24.566	30.796	1.00	31.75
ATOM	1514	CB	VAL	C1026	27.598	21.959	30.748	1.00	29.54
ATOM	1515	CG1	VAL	C1026	28.867	21.451	30.040	1.00	26.68
ATOM	1516	CG2	VAL	C1026	26.960	20.808	31.527	1.00	28.00
ATOM	1517	N	LEU	C1027	27.539	25.107	30.208	1.00	29.76
ATOM	1518	CA	LEU	C1027	27.925	26.331	29.524	1.00	27.25
ATOM	1519	C	LEU	C1027	28.729	27.263	30.410	1.00	25.12
ATOM	1520	O	LEU	C1027	29.764	27.833	30.030	1.00	27.00
ATOM	1521	CB	LEU	C1027	26.664	27.044	28.959	1.00	27.55
ATOM	1522	CG	LEU	C1027	26.904	28.561	28.667	1.00	27.68
ATOM	1523	CD1	LEU	C1027	27.658	28.914	27.434	1.00	28.77
ATOM	1524	CD2	LEU	C1027	25.485	29.174	28.511	1.00	29.96
ATOM	1525	N	LEU	C1028	28.311	27.500	31.665	1.00	27.12
ATOM	1526	CA	LEU	C1028	28.994	28.386	32.576	1.00	26.05
ATOM	1527	C	LEU	C1028	30.399	27.853	32.836	1.00	28.29
ATOM	1528	O	LEU	C1028	31.296	28.666	32.888	1.00	27.74
ATOM	1529	CB	LEU	C1028	28.123	28.576	33.809	1.00	24.95
ATOM	1530	CG	LEU	C1028	28.601	29.349	34.990	1.00	26.00
ATOM	1531	CD1	LEU	C1028	28.932	30.805	34.567	1.00	26.51
ATOM	1532	CD2	LEU	C1028	27.771	29.411	36.264	1.00	23.62
ATOM	1533	N	TRP	C1029	30.569	26.514	32.998	1.00	27.52

FIG. 5AA

ATOM	1534	CA	TRP	C1029	31.811	25.618	33.200	1.00	25.28
ATOM	1535	C	TRP	C1029	32.677	26.052	31.992	1.00	24.21
ATOM	1536	O	TRP	C1029	33.809	26.411	32.199	1.00	28.34
ATOM	1537	CB	TRP	C1029	31.604	24.291	33.488	1.00	25.52
ATOM	1538	CG	TRP	C1029	32.875	23.609	33.873	1.00	23.89
ATOM	1539	CD1	TRP	C1029	33.316	23.467	35.159	1.00	23.77
ATOM	1540	CD2	TRP	C1029	33.901	23.125	33.013	1.00	25.22
ATOM	1541	NE1	TRP	C1029	34.566	22.870	35.125	1.00	28.07
ATOM	1542	CE2	TRP	C1029	34.922	22.645	33.819	1.00	27.51
ATOM	1543	CE3	TRP	C1029	34.013	23.005	31.620	1.00	27.28
ATOM	1544	CZ2	TRP	C1029	36.095	21.998	33.349	1.00	30.61
ATOM	1545	CZ3	TRP	C1029	35.169	22.378	31.126	1.00	30.99
ATOM	1546	CH2	TRP	C1029	36.195	21.931	31.972	1.00	29.91
ATOM	1547	N	GLU	C1030	32.196	26.006	30.773	1.00	22.75
ATOM	1548	CA	GLU	C1030	32.865	26.380	29.590	1.00	24.64
ATOM	1549	C	GLU	C1030	33.291	27.882	29.553	1.00	23.46
ATOM	1550	O	GLU	C1030	34.433	28.114	29.047	1.00	23.61
ATOM	1551	CB	GLU	C1030	32.036	26.144	28.339	1.00	22.23
ATOM	1552	CG	GLU	C1030	31.853	24.671	28.076	1.00	27.85
ATOM	1553	CD	GLU	C1030	30.969	24.399	26.881	1.00	33.40
ATOM	1554	OE1	GLU	C1030	29.767	24.531	27.111	1.00	33.08
ATOM	1555	OE2	GLU	C1030	31.477	24.088	25.792	1.00	37.59
ATOM	1556	N	ILE	C1031	32.413	28.784	30.027	1.00	20.93
ATOM	1557	CA	ILE	C1031	32.888	30.190	29.987	1.00	23.32
ATOM	1558	C	ILE	C1031	34.099	30.417	30.881	1.00	24.20
ATOM	1559	O	ILE	C1031	35.125	31.060	30.547	1.00	25.10
ATOM	1560	CB	ILE	C1031	31.720	31.156	30.365	1.00	22.53
ATOM	1561	CG1	ILE	C1031	30.622	31.066	29.330	1.00	24.20
ATOM	1562	CG2	ILE	C1031	32.262	32.584	30.449	1.00	25.77
ATOM	1563	CD1	ILE	C1031	29.254	31.567	29.766	1.00	24.02
ATOM	1564	N	VAL	C1032	34.002	30.128	32.180	1.00	23.96
ATOM	1565	CA	VAL	C1032	34.923	30.263	33.255	1.00	28.42
ATOM	1566	C	VAL	C1032	36.251	29.547	32.943	1.00	31.87
ATOM	1567	O	VAL	C1032	37.324	30.118	33.157	1.00	31.88
ATOM	1568	CB	VAL	C1032	34.229	29.636	34.479	1.00	31.74
ATOM	1569	CG1	VAL	C1032	35.145	28.990	35.490	1.00	35.56
ATOM	1570	CG2	VAL	C1032	33.241	30.562	35.210	1.00	29.88
ATOM	1571	N	SER	C1033	36.236	28.433	32.262	1.00	29.60
ATOM	1572	CA	SER	C1033	37.352	27.612	31.846	1.00	29.62
ATOM	1573	C	SER	C1033	37.900	28.101	30.520	1.00	30.68
ATOM	1574	O	SER	C1033	38.900	27.598	30.046	1.00	30.21
ATOM	1575	CB	SER	C1033	36.909	26.139	31.703	1.00	30.12
ATOM	1576	OG	SER	C1033	36.408	25.725	30.430	1.00	30.39
ATOM	1577	N	LEU	C1034	37.291	29.100	29.905	1.00	28.42
ATOM	1578	CA	LEU	C1034	37.787	29.635	28.638	1.00	31.98
ATOM	1579	C	LEU	C1034	37.753	28.432	27.688	1.00	32.37
ATOM	1580	O	LEU	C1034	38.731	27.936	27.147	1.00	39.15
ATOM	1581	CB	LEU	C1034	39.205	30.261	28.704	1.00	29.58
ATOM	1582	CG	LEU	C1034	39.466	31.409	29.630	1.00	28.94
ATOM	1583	CD1	LEU	C1034	40.895	31.922	29.656	1.00	30.58
ATOM	1584	CD2	LEU	C1034	38.617	32.636	29.209	1.00	26.58
ATOM	1585	N	GLY	C1035	36.530	27.864	27.544	1.00	28.98
ATOM	1586	CA	GLY	C1035	36.357	26.754	26.647	1.00	24.56
ATOM	1587	C	GLY	C1035	37.171	25.481	26.790	1.00	20.81
ATOM	1588	O	GLY	C1035	37.321	24.796	25.771	1.00	21.90
ATOM	1589	N	GLY	C1036	37.326	24.968	27.997	1.00	21.82
ATOM	1590	CA	GLY	C1036	37.834	23.629	28.239	1.00	25.47

FIG. 5BB

ATOM	1591	C	GLY	C1036	36.727	22.590	27.923	1.00	28.57
ATOM	1592	O	GLY	C1036	35.562	22.944	28.062	1.00	33.09
ATOM	1593	N	THR	C1037	37.098	21.424	27.446	1.00	31.18
ATOM	1594	CA	THR	C1037	36.071	20.402	27.101	1.00	31.40
ATOM	1595	C	THR	C1037	35.671	19.771	28.411	1.00	29.08
ATOM	1596	O	THR	C1037	36.402	19.322	29.267	1.00	28.43
ATOM	1597	CB	THR	C1037	36.849	19.362	26.248	1.00	35.25
ATOM	1598	OG1	THR	C1037	37.143	19.856	24.934	1.00	34.77
ATOM	1599	CG2	THR	C1037	36.056	18.071	26.103	1.00	39.81
ATOM	1600	N	PRO	C1038	34.318	19.849	28.643	1.00	28.79
ATOM	1601	CA	PRO	C1038	33.748	19.251	29.832	1.00	29.26
ATOM	1602	C	PRO	C1038	34.121	17.764	29.891	1.00	30.33
ATOM	1603	O	PRO	C1038	34.045	17.064	28.877	1.00	30.70
ATOM	1604	CB	PRO	C1038	32.262	19.472	29.632	1.00	29.45
ATOM	1605	CG	PRO	C1038	32.146	20.595	28.674	1.00	26.90
ATOM	1606	CD	PRO	C1038	33.290	20.373	27.726	1.00	26.24
ATOM	1607	N	TYR	C1039	34.507	17.239	31.019	1.00	27.10
ATOM	1608	CA	TYR	C1039	34.831	15.865	31.319	1.00	31.51
ATOM	1609	C	TYR	C1039	35.958	15.322	30.451	1.00	33.48
ATOM	1610	O	TYR	C1039	36.068	14.191	29.947	1.00	32.47
ATOM	1611	CB	TYR	C1039	33.590	14.968	31.246	1.00	29.03
ATOM	1612	CG	TYR	C1039	32.355	15.453	31.980	1.00	28.35
ATOM	1613	CD1	TYR	C1039	31.290	15.997	31.247	1.00	27.58
ATOM	1614	CD2	TYR	C1039	32.220	15.368	33.364	1.00	26.44
ATOM	1615	CE1	TYR	C1039	30.142	16.486	31.827	1.00	23.25
ATOM	1616	CE2	TYR	C1039	31.053	15.846	33.969	1.00	25.69
ATOM	1617	CZ	TYR	C1039	30.031	16.398	33.196	1.00	25.31
ATOM	1618	OH	TYR	C1039	28.870	16.776	33.851	1.00	28.82
ATOM	1619	N	CYS	C1040	36.877	16.276	30.243	1.00	37.16
ATOM	1620	CA	CYS	C1040	38.045	16.095	29.389	1.00	38.31
ATOM	1621	C	CYS	C1040	38.733	14.821	29.848	1.00	36.75
ATOM	1622	O	CYS	C1040	38.962	14.593	31.042	1.00	33.37
ATOM	1623	CB	CYS	C1040	38.886	17.360	29.511	1.00	41.12
ATOM	1624	SG	CYS	C1040	40.570	17.157	28.904	1.00	52.08
ATOM	1625	N	GLY	C1041	38.916	13.899	28.920	1.00	38.90
ATOM	1626	CA	GLY	C1041	39.550	12.613	29.230	1.00	43.75
ATOM	1627	C	GLY	C1041	38.531	11.489	29.459	1.00	46.25
ATOM	1628	O	GLY	C1041	38.940	10.313	29.384	1.00	45.71
ATOM	1629	N	MET	C1042	37.288	11.831	29.785	1.00	46.22
ATOM	1630	CA	MET	C1042	36.267	10.832	30.078	1.00	47.06
ATOM	1631	C	MET	C1042	35.471	10.388	28.874	1.00	47.05
ATOM	1632	O	MET	C1042	35.257	11.143	27.937	1.00	47.49
ATOM	1633	CB	MET	C1042	35.281	11.343	31.119	1.00	46.72
ATOM	1634	CG	MET	C1042	35.944	11.646	32.445	1.00	48.06
ATOM	1635	SD	MET	C1042	34.712	11.819	33.734	1.00	51.59
ATOM	1636	CE	MET	C1042	33.816	10.274	33.378	1.00	51.12
ATOM	1637	N	THR	C1043	35.143	9.097	28.852	1.00	48.58
ATOM	1638	CA	THR	C1043	34.359	8.548	27.745	1.00	50.37
ATOM	1639	C	THR	C1043	32.867	8.824	27.938	1.00	49.20
ATOM	1640	O	THR	C1043	32.469	8.990	29.090	1.00	48.53
ATOM	1641	CB	THR	C1043	34.541	7.022	27.715	1.00	49.50
ATOM	1642	OG1	THR	C1043	33.825	6.420	28.780	1.00	49.52
ATOM	1643	CG2	THR	C1043	36.053	6.740	27.911	1.00	48.66
ATOM	1644	N	CYS	C1044	32.090	8.784	26.869	1.00	52.39
ATOM	1645	CA	CYS	C1044	30.591	8.992	27.031	1.00	54.39
ATOM	1646	C	CYS	C1044	30.054	7.913	27.964	1.00	55.34
ATOM	1647	O	CYS	C1044	29.373	8.230	28.952	1.00	56.27

FIG. 5CC

ATOM	1648	CB	CYS	C1044	29.890	9.166	25.699	1.00	54.86
ATOM	1649	SG	CYS	C1044	30.275	10.658	24.717	1.00	54.87
ATOM	1650	N	ALA	C1045	30.546	6.684	27.883	1.00	53.74
ATOM	1651	CA	ALA	C1045	30.276	5.533	28.691	1.00	53.52
ATOM	1652	C	ALA	C1045	30.319	5.704	30.200	1.00	52.95
ATOM	1653	O	ALA	C1045	29.467	5.296	31.022	1.00	52.64
ATOM	1654	CB	ALA	C1045	31.379	4.491	28.321	1.00	54.24
ATOM	1655	N	GLU	C1046	31.440	6.277	30.650	1.00	50.91
ATOM	1656	CA	GLU	C1046	31.637	6.589	32.076	1.00	48.71
ATOM	1657	C	GLU	C1046	30.675	7.673	32.539	1.00	46.60
ATOM	1658	O	GLU	C1046	30.237	7.666	33.717	1.00	44.26
ATOM	1659	CB	GLU	C1046	33.085	7.002	32.314	1.00	49.93
ATOM	1660	CG	GLU	C1046	34.115	6.109	31.628	1.00	53.13
ATOM	1661	CD	GLU	C1046	35.513	6.735	31.729	1.00	54.82
ATOM	1662	OE1	GLU	C1046	36.134	6.539	32.795	1.00	54.82
ATOM	1663	OE2	GLU	C1046	35.963	7.416	30.783	1.00	55.96
ATOM	1664	N	LEU	C1047	30.268	8.586	31.614	1.00	45.34
ATOM	1665	CA	LEU	C1047	29.331	9.632	32.066	1.00	44.07
ATOM	1666	C	LEU	C1047	27.983	9.017	32.439	1.00	42.99
ATOM	1667	O	LEU	C1047	27.530	9.215	33.576	1.00	42.01
ATOM	1668	CB	LEU	C1047	29.181	10.815	31.111	1.00	45.07
ATOM	1669	CG	LEU	C1047	30.430	11.706	30.918	1.00	44.08
ATOM	1670	CD1	LEU	C1047	30.038	12.921	30.115	1.00	45.50
ATOM	1671	CD2	LEU	C1047	31.071	12.058	32.245	1.00	42.85
ATOM	1672	N	TYR	C1048	27.409	8.182	31.588	1.00	43.22
ATOM	1673	CA	TYR	C1048	26.213	7.392	31.910	1.00	44.38
ATOM	1674	C	TYR	C1048	26.397	6.646	33.245	1.00	44.87
ATOM	1675	O	TYR	C1048	25.486	6.717	34.085	1.00	43.82
ATOM	1676	CB	TYR	C1048	25.905	6.343	30.853	1.00	44.96
ATOM	1677	CG	TYR	C1048	25.256	6.871	29.600	1.00	47.81
ATOM	1678	CD1	TYR	C1048	26.033	7.330	28.545	1.00	47.83
ATOM	1679	CD2	TYR	C1048	23.852	6.898	29.482	1.00	48.40
ATOM	1680	CE1	TYR	C1048	25.436	7.802	27.387	1.00	47.27
ATOM	1681	CE2	TYR	C1048	23.246	7.366	28.324	1.00	48.08
ATOM	1682	CZ	TYR	C1048	24.075	7.815	27.294	1.00	48.94
ATOM	1683	OH	TYR	C1048	23.413	8.274	26.168	1.00	49.94
ATOM	1684	N	GLU	C1049	27.591	6.069	33.477	1.00	42.94
ATOM	1685	CA	GLU	C1049	27.749	5.400	34.754	1.00	45.35
ATOM	1686	C	GLU	C1049	28.155	6.333	35.873	1.00	44.67
ATOM	1687	O	GLU	C1049	27.588	6.137	36.975	1.00	45.76
ATOM	1688	CB	GLU	C1049	28.683	4.171	34.686	1.00	47.30
ATOM	1689	CG	GLU	C1049	30.158	4.453	34.837	1.00	49.28
ATOM	1690	CD	GLU	C1049	31.072	3.245	35.050	1.00	50.85
ATOM	1691	OE1	GLU	C1049	31.702	2.810	34.042	1.00	51.60
ATOM	1692	OE2	GLU	C1049	31.179	2.748	36.200	1.00	49.78
ATOM	1693	N	LYS	C1050	29.038	7.320	35.685	1.00	45.45
ATOM	1694	CA	LYS	C1050	29.387	8.148	36.861	1.00	46.05
ATOM	1695	C	LYS	C1050	28.404	9.253	37.175	1.00	44.76
ATOM	1696	O	LYS	C1050	28.099	9.497	38.375	1.00	44.16
ATOM	1697	CB	LYS	C1050	30.814	8.668	36.707	1.00	49.41
ATOM	1698	CG	LYS	C1050	31.798	7.565	36.380	1.00	52.04
ATOM	1699	CD	LYS	C1050	33.285	7.938	36.456	1.00	54.77
ATOM	1700	CE	LYS	C1050	34.086	6.629	36.533	1.00	56.01
ATOM	1701	NZ	LYS	C1050	35.565	6.819	36.433	1.00	58.90
ATOM	1702	N	LEU	C1051	27.733	9.813	36.163	1.00	41.92
ATOM	1703	CA	LEU	C1051	26.746	10.866	36.552	1.00	43.18
ATOM	1704	C	LEU	C1051	25.759	10.435	37.607	1.00	43.39

FIG. 5DD

ATOM	1705	O	LEU	C1051	25.582	11.062	38.662	1.00 43.64
ATOM	1706	CB	LEU	C1051	26.145	11.496	35.307	1.00 43.49
ATOM	1707	CG	LEU	C1051	27.096	12.382	34.480	1.00 42.95
ATOM	1708	CD1	LEU	C1051	26.331	12.985	33.326	1.00 43.01
ATOM	1709	CD2	LEU	C1051	27.702	13.468	35.366	1.00 43.66
ATOM	1710	N	PRO	C1052	25.084	9.288	37.475	1.00 45.02
ATOM	1711	CA	PRO	C1052	24.140	8.817	38.470	1.00 45.84
ATOM	1712	C	PRO	C1052	24.736	8.635	39.839	1.00 47.07
ATOM	1713	O	PRO	C1052	24.088	8.826	40.880	1.00 48.20
ATOM	1714	CB	PRO	C1052	23.559	7.544	37.854	1.00 45.47
ATOM	1715	CG	PRO	C1052	23.652	7.799	36.384	1.00 44.83
ATOM	1716	CD	PRO	C1052	25.013	8.487	36.242	1.00 45.28
ATOM	1717	N	GLN	C1053	26.006	8.296	40.007	1.00 50.49
ATOM	1718	CA	GLN	C1053	26.594	8.130	41.331	1.00 52.45
ATOM	1719	C	GLN	C1053	26.921	9.462	41.976	1.00 51.74
ATOM	1720	O	GLN	C1053	27.231	9.442	43.175	1.00 51.45
ATOM	1721	CB	GLN	C1053	27.798	7.199	41.221	1.00 55.75
ATOM	1722	CG	GLN	C1053	27.411	5.794	40.768	1.00 61.04
ATOM	1723	CD	GLN	C1053	26.526	5.041	41.743	1.00 64.91
ATOM	1724	OE1	GLN	C1053	26.851	4.904	42.948	1.00 66.92
ATOM	1725	NE2	GLN	C1053	25.370	4.528	41.286	1.00 65.52
ATOM	1726	N	GLY	C1054	26.801	10.624	41.320	1.00 49.79
ATOM	1727	CA	GLY	C1054	27.061	11.874	42.052	1.00 46.62
ATOM	1728	C	GLY	C1054	28.276	12.597	41.495	1.00 44.62
ATOM	1729	O	GLY	C1054	28.683	13.662	41.920	1.00 43.65
ATOM	1730	N	TYR	C1055	28.917	12.051	40.482	1.00 45.48
ATOM	1731	CA	TYR	C1055	30.099	12.698	39.937	1.00 45.51
ATOM	1732	C	TYR	C1055	29.685	13.995	39.214	1.00 44.95
ATOM	1733	O	TYR	C1055	28.622	13.976	38.583	1.00 46.39
ATOM	1734	CB	TYR	C1055	30.767	11.776	38.932	1.00 45.73
ATOM	1735	CG	TYR	C1055	32.055	12.414	38.433	1.00 48.52
ATOM	1736	CD1	TYR	C1055	33.235	12.302	39.143	1.00 48.82
ATOM	1737	CD2	TYR	C1055	32.045	13.129	37.234	1.00 48.37
ATOM	1738	CE1	TYR	C1055	34.401	12.898	38.658	1.00 48.87
ATOM	1739	CE2	TYR	C1055	33.178	13.723	36.737	1.00 47.42
ATOM	1740	CZ	TYR	C1055	34.354	13.582	37.459	1.00 49.27
ATOM	1741	OH	TYR	C1055	35.488	14.170	36.952	1.00 48.77
ATOM	1742	N	ARG	C1056	30.485	15.051	39.252	1.00 40.28
ATOM	1743	CA	ARG	C1056	30.189	16.276	38.566	1.00 38.71
ATOM	1744	C	ARG	C1056	31.481	17.012	38.176	1.00 39.85
ATOM	1745	O	ARG	C1056	32.472	16.797	38.879	1.00 42.11
ATOM	1746	CB	ARG	C1056	29.407	17.281	39.408	1.00 38.04
ATOM	1747	CG	ARG	C1056	27.996	17.004	39.890	1.00 37.78
ATOM	1748	CD	ARG	C1056	27.022	16.584	38.810	1.00 34.37
ATOM	1749	NE	ARG	C1056	25.677	16.380	39.370	1.00 32.75
ATOM	1750	CZ	ARG	C1056	25.172	15.135	39.461	1.00 34.13
ATOM	1751	NH1	ARG	C1056	23.934	15.014	39.951	1.00 33.89
ATOM	1752	NH2	ARG	C1056	25.884	14.083	39.063	1.00 31.70
ATOM	1753	N	LEU	C1057	31.450	17.843	37.130	1.00 37.74
ATOM	1754	CA	LEU	C1057	32.615	18.640	36.829	1.00 38.61
ATOM	1755	C	LEU	C1057	33.280	19.260	38.062	1.00 37.18
ATOM	1756	O	LEU	C1057	32.759	19.829	39.007	1.00 36.18
ATOM	1757	CB	LEU	C1057	32.223	19.785	35.886	1.00 39.58
ATOM	1758	CG	LEU	C1057	31.870	19.236	34.492	1.00 40.26
ATOM	1759	CD1	LEU	C1057	31.190	20.384	33.790	1.00 41.53
ATOM	1760	CD2	LEU	C1057	33.089	18.719	33.746	1.00 40.04
ATOM	1761	N	GLU	C1058	34.597	19.231	37.962	1.00 38.47

FIG. 5EE

ATOM	1762	CA	GLU	C1058	35.494	19.715	39.003	1.00	40.99
ATOM	1763	C	GLU	C1058	35.655	21.237	38.941	1.00	37.60
ATOM	1764	O	GLU	C1058	35.665	21.759	37.841	1.00	37.18
ATOM	1765	CB	GLU	C1058	36.808	18.952	38.778	1.00	43.93
ATOM	1766	CG	GLU	C1058	37.256	18.728	37.367	1.00	49.34
ATOM	1767	CD	GLU	C1058	36.540	18.005	36.265	1.00	51.18
ATOM	1768	OE1	GLU	C1058	36.581	18.538	35.121	1.00	50.19
ATOM	1769	OE2	GLU	C1058	35.931	16.902	36.361	1.00	52.82
ATOM	1770	N	LYS	C1059	35.708	21.975	40.005	1.00	35.88
ATOM	1771	CA	LYS	C1059	35.948	23.424	39.950	1.00	40.12
ATOM	1772	C	LYS	C1059	37.345	23.831	39.473	1.00	41.54
ATOM	1773	O	LYS	C1059	38.332	23.431	40.095	1.00	41.88
ATOM	1774	CB	LYS	C1059	35.946	23.896	41.417	1.00	39.21
ATOM	1775	CG	LYS	C1059	35.984	25.413	41.569	1.00	41.97
ATOM	1776	CD	LYS	C1059	35.953	25.810	43.048	1.00	43.62
ATOM	1777	CE	LYS	C1059	37.349	25.786	43.641	1.00	43.92
ATOM	1778	NZ	LYS	C1059	38.192	26.906	43.099	1.00	44.39
ATOM	1779	N	PRO	C1060	37.498	24.651	38.439	1.00	41.99
ATOM	1780	CA	PRO	C1060	38.795	25.166	38.040	1.00	42.27
ATOM	1781	C	PRO	C1060	39.441	25.920	39.186	1.00	42.45
ATOM	1782	O	PRO	C1060	38.840	26.618	39.996	1.00	40.76
ATOM	1783	CB	PRO	C1060	38.529	26.115	36.894	1.00	43.06
ATOM	1784	CG	PRO	C1060	37.145	25.765	36.416	1.00	41.60
ATOM	1785	CD	PRO	C1060	36.408	25.170	37.589	1.00	41.74
ATOM	1786	N	LEU	C1061	40.773	25.843	39.287	1.00	44.11
ATOM	1787	CA	LEU	C1061	41.557	26.440	40.325	1.00	44.84
ATOM	1788	C	LEU	C1061	41.416	27.941	40.443	1.00	44.71
ATOM	1789	O	LEU	C1061	41.441	28.470	41.567	1.00	45.26
ATOM	1790	CB	LEU	C1061	43.036	26.089	40.055	1.00	48.79
ATOM	1791	CG	LEU	C1061	43.314	24.624	40.459	1.00	52.11
ATOM	1792	CD1	LEU	C1061	44.673	24.204	39.897	1.00	53.08
ATOM	1793	CD2	LEU	C1061	43.288	24.512	41.984	1.00	52.05
ATOM	1794	N	ASN	C1062	41.247	28.623	39.321	1.00	44.44
ATOM	1795	CA	ASN	C1062	41.112	30.085	39.327	1.00	44.45
ATOM	1796	C	ASN	C1062	39.661	30.582	39.363	1.00	44.24
ATOM	1797	O	ASN	C1062	39.394	31.757	39.073	1.00	42.70
ATOM	1798	CB	ASN	C1062	41.811	30.536	38.059	1.00	47.14
ATOM	1799	CG	ASN	C1062	41.018	30.280	36.799	1.00	50.71
ATOM	1800	OD1	ASN	C1062	40.297	29.260	36.680	1.00	55.26
ATOM	1801	ND2	ASN	C1062	41.160	31.208	35.873	1.00	49.84
ATOM	1802	N	CYS	C1063	38.727	29.727	39.787	1.00	40.21
ATOM	1803	CA	CYS	C1063	37.312	30.006	39.917	1.00	39.16
ATOM	1804	C	CYS	C1063	36.922	30.226	41.375	1.00	40.26
ATOM	1805	O	CYS	C1063	37.149	29.298	42.177	1.00	38.11
ATOM	1806	CB	CYS	C1063	36.476	28.796	39.430	1.00	36.02
ATOM	1807	SG	CYS	C1063	34.684	29.162	39.283	1.00	36.25
ATOM	1808	N	ASP	C1064	36.179	31.287	41.675	1.00	39.98
ATOM	1809	CA	ASP	C1064	35.704	31.514	43.034	1.00	42.23
ATOM	1810	C	ASP	C1064	34.623	30.474	43.367	1.00	43.63
ATOM	1811	O	ASP	C1064	33.885	29.998	42.516	1.00	42.13
ATOM	1812	CB	ASP	C1064	35.166	32.915	43.277	1.00	44.24
ATOM	1813	CG	ASP	C1064	34.744	33.348	44.660	1.00	47.38
ATOM	1814	OD1	ASP	C1064	35.591	34.016	45.335	1.00	49.14
ATOM	1815	OD2	ASP	C1064	33.594	33.165	45.169	1.00	46.30
ATOM	1816	N	ASP	C1065	34.571	30.128	44.646	1.00	44.20
ATOM	1817	CA	ASP	C1065	33.681	29.213	45.285	1.00	46.41
ATOM	1818	C	ASP	C1065	32.214	29.629	45.059	1.00	46.09

FIG. 5FF

ATOM	1819	O	ASP	C1065	31.383	28.772	44.807	1.00	45.90
ATOM	1820	CB	ASP	C1065	33.999	29.111	46.780	1.00	49.84
ATOM	1821	CG	ASP	C1065	34.972	28.020	47.179	1.00	54.04
ATOM	1822	OD1	ASP	C1065	35.370	27.139	46.384	1.00	54.54
ATOM	1823	OD2	ASP	C1065	35.412	27.941	48.364	1.00	56.55
ATOM	1824	N	GLU	C1066	31.930	30.931	44.991	1.00	46.33
ATOM	1825	CA	GLU	C1066	30.585	31.364	44.699	1.00	46.37
ATOM	1826	C	GLU	C1066	30.162	30.946	43.279	1.00	43.58
ATOM	1827	O	GLU	C1066	28.974	30.622	43.161	1.00	40.53
ATOM	1828	CB	GLU	C1066	30.362	32.870	44.901	1.00	47.78
ATOM	1829	CG	GLU	C1066	30.464	33.371	46.327	1.00	51.27
ATOM	1830	CD	GLU	C1066	30.147	34.853	46.483	1.00	54.46
ATOM	1831	OE1	GLU	C1066	30.977	35.632	47.023	1.00	56.49
ATOM	1832	OE2	GLU	C1066	29.039	35.278	46.075	1.00	54.91
ATOM	1833	N	VAL	C1067	31.031	31.026	42.267	1.00	40.02
ATOM	1834	CA	VAL	C1067	30.592	30.670	40.914	1.00	38.39
ATOM	1835	C	VAL	C1067	30.361	29.166	40.750	1.00	38.56
ATOM	1836	O	VAL	C1067	29.492	28.741	39.975	1.00	35.01
ATOM	1837	CB	VAL	C1067	31.561	31.094	39.797	1.00	37.83
ATOM	1838	CG1	VAL	C1067	31.071	30.760	38.416	1.00	34.84
ATOM	1839	CG2	VAL	C1067	31.809	32.609	39.878	1.00	39.35
ATOM	1840	N	TYR	C1068	31.258	28.419	41.393	1.00	37.89
ATOM	1841	CA	TYR	C1068	31.203	26.969	41.346	1.00	38.97
ATOM	1842	C	TYR	C1068	29.924	26.510	42.044	1.00	40.70
ATOM	1843	O	TYR	C1068	29.265	25.613	41.492	1.00	38.63
ATOM	1844	CB	TYR	C1068	32.437	26.278	41.913	1.00	37.20
ATOM	1845	CG	TYR	C1068	32.470	24.770	41.798	1.00	35.05
ATOM	1846	CD1	TYR	C1068	32.535	24.158	40.556	1.00	34.59
ATOM	1847	CD2	TYR	C1068	32.431	23.934	42.903	1.00	35.51
ATOM	1848	CE1	TYR	C1068	32.536	22.785	40.405	1.00	33.51
ATOM	1849	CE2	TYR	C1068	32.456	22.549	42.800	1.00	33.38
ATOM	1850	CZ	TYR	C1068	32.540	22.006	41.540	1.00	33.70
ATOM	1851	OH	TYR	C1068	32.545	20.637	41.342	1.00	37.05
ATOM	1852	N	ASP	C1069	29.573	27.177	43.159	1.00	42.06
ATOM	1853	CA	ASP	C1069	28.316	26.862	43.806	1.00	42.68
ATOM	1854	C	ASP	C1069	27.124	27.069	42.869	1.00	40.99
ATOM	1855	O	ASP	C1069	26.233	26.193	42.884	1.00	40.08
ATOM	1856	CB	ASP	C1069	28.116	27.676	45.094	1.00	47.98
ATOM	1857	CG	ASP	C1069	28.983	27.092	46.212	1.00	53.70
ATOM	1858	OD1	ASP	C1069	29.487	25.940	46.045	1.00	55.80
ATOM	1859	OD2	ASP	C1069	29.161	27.786	47.254	1.00	55.99
ATOM	1860	N	LEU	C1070	27.080	28.150	42.087	1.00	36.81
ATOM	1861	CA	LEU	C1070	25.977	28.308	41.140	1.00	36.03
ATOM	1862	C	LEU	C1070	25.905	27.172	40.123	1.00	34.83
ATOM	1863	O	LEU	C1070	24.833	26.703	39.743	1.00	32.57
ATOM	1864	CB	LEU	C1070	26.131	29.666	40.472	1.00	33.68
ATOM	1865	CG	LEU	C1070	25.095	30.113	39.458	1.00	35.12
ATOM	1866	CD1	LEU	C1070	23.674	29.955	40.003	1.00	34.71
ATOM	1867	CD2	LEU	C1070	25.391	31.582	39.084	1.00	34.63
ATOM	1868	N	MET	C1071	27.036	26.703	39.602	1.00	36.71
ATOM	1869	CA	MET	C1071	27.131	25.568	38.706	1.00	37.17
ATOM	1870	C	MET	C1071	26.555	24.302	39.372	1.00	36.93
ATOM	1871	O	MET	C1071	25.808	23.574	38.735	1.00	36.82
ATOM	1872	CB	MET	C1071	28.569	25.145	38.294	1.00	35.35
ATOM	1873	CG	MET	C1071	29.354	26.145	37.465	1.00	35.64
ATOM	1874	SD	MET	C1071	31.096	25.645	37.207	1.00	32.11
ATOM	1875	CE	MET	C1071	31.839	27.209	36.753	1.00	34.27

FIG. 5GG

ATOM	1876	N	ARG	C1072	26.959	23.943	40.580	1.00	36.71
ATOM	1877	CA	ARG	C1072	26.550	22.771	41.323	1.00	37.27
ATOM	1878	C	ARG	C1072	25.039	22.687	41.557	1.00	36.15
ATOM	1879	O	ARG	C1072	24.384	21.638	41.587	1.00	37.31
ATOM	1880	CB	ARG	C1072	27.272	22.810	42.713	1.00	39.01
ATOM	1881	CG	ARG	C1072	28.773	22.514	42.664	1.00	38.84
ATOM	1882	CD	ARG	C1072	29.110	21.260	41.887	1.00	40.99
ATOM	1883	NE	ARG	C1072	28.618	20.088	42.608	1.00	45.98
ATOM	1884	CZ	ARG	C1072	29.217	19.090	43.239	1.00	46.52
ATOM	1885	NH1	ARG	C1072	30.532	18.968	43.255	1.00	44.60
ATOM	1886	NH2	ARG	C1072	28.428	18.173	43.842	1.00	46.54
ATOM	1887	N	GLN	C1073	24.427	23.832	41.775	1.00	36.36
ATOM	1888	CA	GLN	C1073	22.986	24.010	41.934	1.00	36.84
ATOM	1889	C	GLN	C1073	22.289	23.680	40.612	1.00	35.17
ATOM	1890	O	GLN	C1073	21.240	23.043	40.616	1.00	36.12
ATOM	1891	CB	GLN	C1073	22.690	25.436	42.324	1.00	40.62
ATOM	1892	CG	GLN	C1073	22.926	25.928	43.737	1.00	44.26
ATOM	1893	CD	GLN	C1073	22.601	27.425	43.797	1.00	48.97
ATOM	1894	OE1	GLN	C1073	22.895	28.160	44.746	1.00	50.88
ATOM	1895	NE2	GLN	C1073	21.954	27.977	42.770	1.00	50.58
ATOM	1896	N	CYS	C1074	22.888	23.925	39.463	1.00	34.02
ATOM	1897	CA	CYS	C1074	22.346	23.554	38.175	1.00	33.44
ATOM	1898	C	CYS	C1074	22.300	22.048	37.953	1.00	32.85
ATOM	1899	O	CYS	C1074	21.595	21.573	37.050	1.00	28.15
ATOM	1900	CB	CYS	C1074	23.165	24.222	37.052	1.00	32.80
ATOM	1901	SG	CYS	C1074	22.926	26.054	36.945	1.00	29.54
ATOM	1902	N	TRP	C1075	23.155	21.300	38.651	1.00	34.38
ATOM	1903	CA	TRP	C1075	23.323	19.869	38.394	1.00	36.36
ATOM	1904	C	TRP	C1075	22.772	19.008	39.538	1.00	37.35
ATOM	1905	O	TRP	C1075	23.378	17.961	39.809	1.00	36.14
ATOM	1906	CB	TRP	C1075	24.797	19.516	38.184	1.00	31.61
ATOM	1907	CG	TRP	C1075	25.554	20.319	37.170	1.00	32.01
ATOM	1908	CD1	TRP	C1075	25.035	20.735	35.945	1.00	30.72
ATOM	1909	CD2	TRP	C1075	26.905	20.792	37.215	1.00	27.71
ATOM	1910	NE1	TRP	C1075	26.028	21.458	35.263	1.00	27.75
ATOM	1911	CE2	TRP	C1075	27.165	21.473	36.015	1.00	27.79
ATOM	1912	CE3	TRP	C1075	27.923	20.731	38.161	1.00	29.11
ATOM	1913	CZ2	TRP	C1075	28.393	22.095	35.707	1.00	27.12
ATOM	1914	CZ3	TRP	C1075	29.172	21.338	37.861	1.00	27.92
ATOM	1915	CH2	TRP	C1075	29.394	22.010	36.640	1.00	26.04
ATOM	1916	N	ARG	C1076	21.729	19.503	40.206	1.00	38.82
ATOM	1917	CA	ARG	C1076	21.190	18.763	41.348	1.00	40.61
ATOM	1918	C	ARG	C1076	20.509	17.546	40.743	1.00	40.05
ATOM	1919	O	ARG	C1076	19.967	17.688	39.634	1.00	40.43
ATOM	1920	CB	ARG	C1076	20.272	19.608	42.208	1.00	42.35
ATOM	1921	CG	ARG	C1076	20.932	20.378	43.334	1.00	45.64
ATOM	1922	CD	ARG	C1076	20.106	21.505	43.893	1.00	49.70
ATOM	1923	NE	ARG	C1076	20.769	22.441	44.800	1.00	52.00
ATOM	1924	CZ	ARG	C1076	20.478	23.723	45.050	1.00	51.66
ATOM	1925	NH1	ARG	C1076	19.508	24.410	44.455	1.00	50.03
ATOM	1926	NH2	ARG	C1076	21.238	24.353	45.949	1.00	52.86
ATOM	1927	N	GLU	C1077	20.598	16.392	41.374	1.00	41.20
ATOM	1928	CA	GLU	C1077	19.944	15.200	40.818	1.00	42.65
ATOM	1929	C	GLU	C1077	18.447	15.393	40.555	1.00	38.60
ATOM	1930	O	GLU	C1077	17.929	15.043	39.481	1.00	35.94
ATOM	1931	CB	GLU	C1077	20.198	13.968	41.695	1.00	45.87
ATOM	1932	CG	GLU	C1077	20.013	12.643	40.962	1.00	50.08

FIG. 5HH

ATOM	1933	CD	GLU	C1077	20.183	11.401	41.819	1.00	54.47
ATOM	1934	OE1	GLU	C1077	20.561	10.312	41.308	1.00	57.69
ATOM	1935	OE2	GLU	C1077	19.955	11.404	43.055	1.00	56.30
ATOM	1936	N	LYS	C1078	17.706	15.887	41.503	1.00	39.48
ATOM	1937	CA	LYS	C1078	16.243	16.090	41.262	1.00	40.94
ATOM	1938	C	LYS	C1078	16.079	17.369	40.455	1.00	40.21
ATOM	1939	O	LYS	C1078	16.480	18.449	40.854	1.00	38.01
ATOM	1940	CB	LYS	C1078	15.475	16.240	42.568	1.00	43.70
ATOM	1941	CG	LYS	C1078	15.629	15.188	43.605	1.00	46.67
ATOM	1942	CD	LYS	C1078	15.384	15.538	45.015	1.00	49.04
ATOM	1943	CE	LYS	C1078	15.414	14.237	45.826	1.00	53.53
ATOM	1944	NZ	LYS	C1078	14.894	14.422	47.213	1.00	55.30
ATOM	1945	N	PRO	C1079	15.476	17.282	39.286	1.00	38.88
ATOM	1946	CA	PRO	C1079	15.298	18.465	38.451	1.00	39.64
ATOM	1947	C	PRO	C1079	14.654	19.621	39.182	1.00	40.23
ATOM	1948	O	PRO	C1079	15.091	20.778	39.078	1.00	39.41
ATOM	1949	CB	PRO	C1079	14.521	17.924	37.259	1.00	36.96
ATOM	1950	CG	PRO	C1079	14.929	16.461	37.199	1.00	35.65
ATOM	1951	CD	PRO	C1079	14.988	16.035	38.647	1.00	36.92
ATOM	1952	N	TYR	C1080	13.657	19.387	40.028	1.00	41.92
ATOM	1953	CA	TYR	C1080	12.882	20.406	40.717	1.00	43.85
ATOM	1954	C	TYR	C1080	13.587	21.140	41.824	1.00	43.51
ATOM	1955	O	TYR	C1080	13.109	22.140	42.388	1.00	43.12
ATOM	1956	CB	TYR	C1080	11.505	19.831	41.176	1.00	45.60
ATOM	1957	CG	TYR	C1080	11.697	18.722	42.194	1.00	47.84
ATOM	1958	CD1	TYR	C1080	11.973	18.993	43.531	1.00	49.35
ATOM	1959	CD2	TYR	C1080	11.636	17.389	41.798	1.00	49.13
ATOM	1960	CE1	TYR	C1080	12.146	17.958	44.445	1.00	50.14
ATOM	1961	CE2	TYR	C1080	11.806	16.370	42.704	1.00	50.24
ATOM	1962	CZ	TYR	C1080	12.058	16.656	44.030	1.00	50.60
ATOM	1963	OH	TYR	C1080	12.242	15.597	44.908	1.00	53.21
ATOM	1964	N	GLU	C1081	14.799	20.700	42.144	1.00	44.60
ATOM	1965	CA	GLU	C1081	15.638	21.430	43.102	1.00	44.07
ATOM	1966	C	GLU	C1081	16.559	22.432	42.419	1.00	40.19
ATOM	1967	O	GLU	C1081	17.250	23.137	43.126	1.00	37.60
ATOM	1968	CB	GLU	C1081	16.508	20.467	43.922	1.00	45.52
ATOM	1969	CG	GLU	C1081	15.648	19.808	45.014	1.00	50.79
ATOM	1970	CD	GLU	C1081	16.627	18.944	45.789	1.00	54.16
ATOM	1971	OE1	GLU	C1081	16.879	19.248	46.968	1.00	58.46
ATOM	1972	OE2	GLU	C1081	17.210	17.991	45.250	1.00	55.69
ATOM	1973	N	ARG	C1082	16.647	22.458	41.105	1.00	39.28
ATOM	1974	CA	ARG	C1082	17.497	23.363	40.367	1.00	37.58
ATOM	1975	C	ARG	C1082	16.828	24.740	40.394	1.00	38.63
ATOM	1976	O	ARG	C1082	15.612	24.910	40.383	1.00	40.38
ATOM	1977	CB	ARG	C1082	17.704	22.926	38.895	1.00	36.08
ATOM	1978	CG	ARG	C1082	18.469	21.599	38.779	1.00	36.20
ATOM	1979	CD	ARG	C1082	18.609	20.955	37.417	1.00	33.59
ATOM	1980	NE	ARG	C1082	18.832	19.501	37.535	1.00	34.00
ATOM	1981	CZ	ARG	C1082	18.469	18.515	36.714	1.00	32.08
ATOM	1982	NH1	ARG	C1082	17.822	18.762	35.569	1.00	31.72
ATOM	1983	NH2	ARG	C1082	18.708	17.204	36.908	1.00	31.86
ATOM	1984	N	PRO	C1083	17.667	25.772	40.289	1.00	34.94
ATOM	1985	CA	PRO	C1083	17.201	27.135	40.253	1.00	32.78
ATOM	1986	C	PRO	C1083	16.556	27.432	38.912	1.00	33.70
ATOM	1987	O	PRO	C1083	16.641	26.652	37.947	1.00	31.92
ATOM	1988	CB	PRO	C1083	18.446	28.006	40.398	1.00	27.76
ATOM	1989	CG	PRO	C1083	19.621	27.077	40.186	1.00	30.28

FIG. 5II

ATOM	1990	CD	PRO	C1083	19.139	25.661	40.404	1.00	32.35
ATOM	1991	N	SER	C1084	15.816	28.558	38.933	1.00	31.68
ATOM	1992	CA	SER	C1084	15.199	29.032	37.705	1.00	31.93
ATOM	1993	C	SER	C1084	16.210	30.014	37.080	1.00	31.48
ATOM	1994	O	SER	C1084	17.144	30.514	37.733	1.00	29.39
ATOM	1995	CB	SER	C1084	13.873	29.704	38.085	1.00	31.83
ATOM	1996	OG	SER	C1084	14.132	31.022	38.595	1.00	32.90
ATOM	1997	N	PHE	C1085	16.099	30.275	35.783	1.00	30.49
ATOM	1998	CA	PHE	C1085	16.882	31.203	35.046	1.00	31.87
ATOM	1999	C	PHE	C1085	16.731	32.620	35.612	1.00	35.04
ATOM	2000	O	PHE	C1085	17.778	33.269	35.568	1.00	34.20
ATOM	2001	CB	PHE	C1085	16.631	31.270	33.533	1.00	29.72
ATOM	2002	CG	PHE	C1085	17.113	30.035	32.829	1.00	29.58
ATOM	2003	CD1	PHE	C1085	16.278	29.113	32.259	1.00	27.05
ATOM	2004	CD2	PHE	C1085	18.513	29.847	32.765	1.00	28.92
ATOM	2005	CE1	PHE	C1085	16.764	28.002	31.606	1.00	29.03
ATOM	2006	CE2	PHE	C1085	18.999	28.739	32.078	1.00	31.04
ATOM	2007	CZ	PHE	C1085	18.172	27.810	31.537	1.00	29.42
ATOM	2008	N	ALA	C1086	15.538	32.967	36.152	1.00	34.52
ATOM	2009	CA	ALA	C1086	15.461	34.251	36.811	1.00	36.36
ATOM	2010	C	ALA	C1086	16.330	34.297	38.053	1.00	35.05
ATOM	2011	O	ALA	C1086	16.940	35.370	38.305	1.00	33.03
ATOM	2012	CB	ALA	C1086	13.991	34.579	37.178	1.00	36.02
ATOM	2013	N	GLN	C1087	16.403	33.210	38.808	1.00	34.48
ATOM	2014	CA	GLN	C1087	17.187	33.187	40.043	1.00	37.34
ATOM	2015	C	GLN	C1087	18.692	33.172	39.718	1.00	36.23
ATOM	2016	O	GLN	C1087	19.488	33.831	40.397	1.00	34.12
ATOM	2017	CB	GLN	C1087	16.898	31.991	40.963	1.00	39.18
ATOM	2018	CG	GLN	C1087	15.465	31.766	41.372	1.00	41.60
ATOM	2019	CD	GLN	C1087	15.181	30.507	42.185	1.00	41.95
ATOM	2020	OE1	GLN	C1087	14.644	30.647	43.307	1.00	43.26
ATOM	2021	NE2	GLN	C1087	15.463	29.299	41.755	1.00	38.28
ATOM	2022	N	ILE	C1088	19.023	32.489	38.609	1.00	36.91
ATOM	2023	CA	ILE	C1088	20.421	32.470	38.143	1.00	34.98
ATOM	2024	C	ILE	C1088	20.850	33.891	37.730	1.00	36.64
ATOM	2025	O	ILE	C1088	21.994	34.310	37.999	1.00	38.60
ATOM	2026	CB	ILE	C1088	20.707	31.497	37.017	1.00	31.65
ATOM	2027	CG1	ILE	C1088	20.729	30.014	37.479	1.00	28.80
ATOM	2028	CG2	ILE	C1088	22.108	31.715	36.417	1.00	32.45
ATOM	2029	CD1	ILE	C1088	20.354	29.149	36.296	1.00	24.89
ATOM	2030	N	LEU	C1089	20.006	34.626	37.037	1.00	36.93
ATOM	2031	CA	LEU	C1089	20.288	36.010	36.641	1.00	38.78
ATOM	2032	C	LEU	C1089	20.504	36.934	37.835	1.00	39.65
ATOM	2033	O	LEU	C1089	21.396	37.812	37.840	1.00	38.19
ATOM	2034	CB	LEU	C1089	19.192	36.562	35.727	1.00	39.78
ATOM	2035	CG	LEU	C1089	19.421	37.938	35.087	1.00	41.64
ATOM	2036	CD1	LEU	C1089	20.497	37.892	34.014	1.00	39.98
ATOM	2037	CD2	LEU	C1089	18.113	38.470	34.492	1.00	40.00
ATOM	2038	N	VAL	C1090	19.730	36.740	38.902	1.00	41.42
ATOM	2039	CA	VAL	C1090	19.894	37.611	40.075	1.00	43.28
ATOM	2040	C	VAL	C1090	21.247	37.342	40.727	1.00	43.77
ATOM	2041	O	VAL	C1090	21.948	38.289	41.115	1.00	45.25
ATOM	2042	CB	VAL	C1090	18.759	37.424	41.081	1.00	44.41
ATOM	2043	CG1	VAL	C1090	19.139	38.123	42.387	1.00	45.32
ATOM	2044	CG2	VAL	C1090	17.422	37.989	40.595	1.00	45.38
ATOM	2045	N	SER	C1091	21.634	36.074	40.924	1.00	43.36
ATOM	2046	CA	SER	C1091	22.921	35.817	41.543	1.00	45.59

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ATOM   2047  C   SER C1091      24.044  36.357  40.663  1.00 43.29
ATOM   2048  O   SER C1091      24.987  36.921  41.231  1.00 43.04
ATOM   2049  CB  SER C1091      23.056  34.332  41.946  1.00 48.54
ATOM   2050  OG  SER C1091      22.563  33.588  40.846  1.00 54.84
ATOM   2051  N   LEU C1092      23.971  36.337  39.335  1.00 38.97
ATOM   2052  CA  LEU C1092      25.098  36.849  38.570  1.00 37.84
ATOM   2053  C   LEU C1092      25.118  38.383  38.604  1.00 39.82
ATOM   2054  O   LEU C1092      26.207  38.957  38.627  1.00 35.95
ATOM   2055  CB  LEU C1092      25.098  36.309  37.150  1.00 35.04
ATOM   2056  CG  LEU C1092      25.301  34.789  36.982  1.00 33.88
ATOM   2057  CD1 LEU C1092      24.655  34.383  35.662  1.00 33.07
ATOM   2058  CD2 LEU C1092      26.773  34.446  37.016  1.00 34.04
ATOM   2059  N   ASN C1093      23.942  39.039  38.597  1.00 41.48
ATOM   2060  CA  ASN C1093      23.920  40.525  38.641  1.00 43.61
ATOM   2061  C   ASN C1093      24.527  41.074  39.936  1.00 44.92
ATOM   2062  O   ASN C1093      25.166  42.135  39.946  1.00 44.64
ATOM   2063  CB  ASN C1093      22.509  41.084  38.434  1.00 42.95
ATOM   2064  CG  ASN C1093      21.996  41.095  37.021  1.00 44.32
ATOM   2065  OD1 ASN C1093      20.771  41.140  36.726  1.00 46.00
ATOM   2066  ND2 ASN C1093      22.859  41.098  36.023  1.00 43.94
ATOM   2067  N   ARG C1094      24.374  40.336  41.043  1.00 46.27
ATOM   2068  CA  ARG C1094      24.957  40.724  42.334  1.00 47.34
ATOM   2069  C   ARG C1094      26.473  40.529  42.302  1.00 47.18
ATOM   2070  O   ARG C1094      27.308  41.386  42.683  1.00 48.73
ATOM   2071  CB  ARG C1094      24.207  39.952  43.397  1.00 48.52
ATOM   2072  CG  ARG C1094      24.600  40.135  44.831  1.00 53.04
ATOM   2073  CD  ARG C1094      25.893  39.506  45.266  1.00 55.51
ATOM   2074  NE  ARG C1094      25.811  38.266  46.057  1.00 58.34
ATOM   2075  CZ  ARG C1094      26.945  37.595  46.345  1.00 58.94
ATOM   2076  NH1 ARG C1094      28.144  37.993  45.942  1.00 58.67
ATOM   2077  NH2 ARG C1094      26.892  36.486  47.071  1.00 60.47
ATOM   2078  N   MET C1095      26.945  39.465  41.654  1.00 43.61
ATOM   2079  CA  MET C1095      28.378  39.288  41.439  1.00 41.53
ATOM   2080  C   MET C1095      28.854  40.419  40.535  1.00 37.96
ATOM   2081  O   MET C1095      29.993  40.855  40.670  1.00 39.00
ATOM   2082  CB  MET C1095      28.772  37.969  40.755  1.00 39.83
ATOM   2083  CG  MET C1095      28.636  36.767  41.644  1.00 42.24
ATOM   2084  SD  MET C1095      28.588  35.160  40.819  1.00 43.52
ATOM   2085  CE  MET C1095      29.492  34.284  42.084  1.00 43.64
ATOM   2086  N   LEU C1096      28.128  40.770  39.489  1.00 38.63
ATOM   2087  CA  LEU C1096      28.592  41.811  38.583  1.00 40.32
ATOM   2088  C   LEU C1096      28.726  43.159  39.300  1.00 45.56
ATOM   2089  O   LEU C1096      29.676  43.913  39.027  1.00 43.98
ATOM   2090  CB  LEU C1096      27.705  41.881  37.363  1.00 38.78
ATOM   2091  CG  LEU C1096      27.859  40.853  36.254  1.00 36.87
ATOM   2092  CD1 LEU C1096      26.623  40.917  35.364  1.00 37.20
ATOM   2093  CD2 LEU C1096      29.157  41.041  35.484  1.00 36.07
ATOM   2094  N   GLU C1097      27.840  43.531  40.207  1.00 50.71
ATOM   2095  CA  GLU C1097      27.911  44.809  40.888  1.00 56.21
ATOM   2096  C   GLU C1097      28.997  45.073  41.913  1.00 57.95
ATOM   2097  O   GLU C1097      29.115  46.249  42.308  1.00 58.26
ATOM   2098  CB  GLU C1097      26.511  45.083  41.496  1.00 59.17
ATOM   2099  CG  GLU C1097      25.588  45.556  40.362  1.00 62.97
ATOM   2100  CD  GLU C1097      25.880  46.999  39.984  1.00 65.89
ATOM   2101  OE1 GLU C1097      26.772  47.604  40.633  1.00 67.34
ATOM   2102  OE2 GLU C1097      25.159  47.465  39.064  1.00 68.13
ATOM   2103  N   GLU C1098      29.832  44.134  42.340  1.00 59.64
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FIG. 5KK

ATOM	2104	CA	GLU	C1098	30.923	44.413	43.251	1.00	62.30
ATOM	2105	C	GLU	C1098	32.317	44.135	42.709	1.00	61.47
ATOM	2106	O	GLU	C1098	32.699	43.098	42.165	1.00	63.11
ATOM	2107	CB	GLU	C1098	30.721	43.618	44.546	1.00	63.71
ATOM	2108	CG	GLU	C1098	30.447	42.141	44.289	1.00	64.85
ATOM	2109	CD	GLU	C1098	30.147	41.457	45.616	1.00	66.52
ATOM	2110	OE1	GLU	C1098	29.135	41.807	46.262	1.00	67.90
ATOM	2111	OE2	GLU	C1098	30.943	40.587	46.021	1.00	67.37
ATOM	2112	N	ARG	C1099	33.234	45.047	43.011	1.00	62.10
ATOM	2113	CA	ARG	C1099	34.637	45.044	42.675	1.00	60.00
ATOM	2114	C	ARG	C1099	35.404	43.736	42.782	1.00	58.76
ATOM	2115	O	ARG	C1099	36.433	43.655	42.072	1.00	60.07
ATOM	2116	CB	ARG	C1099	35.327	46.048	43.623	1.00	61.21
ATOM	2117	N	LYS	C1100	35.024	42.747	43.594	1.00	56.32
ATOM	2118	CA	LYS	C1100	35.843	41.536	43.624	1.00	55.34
ATOM	2119	C	LYS	C1100	35.881	40.863	42.258	1.00	53.59
ATOM	2120	O	LYS	C1100	35.083	41.060	41.366	1.00	53.08
ATOM	2121	CB	LYS	C1100	35.416	40.629	44.760	1.00	56.50
ATOM	2122	CG	LYS	C1100	34.580	39.418	44.451	1.00	57.25
ATOM	2123	CD	LYS	C1100	33.972	38.745	45.669	1.00	57.47
ATOM	2124	CE	LYS	C1100	34.923	37.780	46.342	1.00	59.43
ATOM	2125	NZ	LYS	C1100	34.265	36.502	46.768	1.00	59.87
ATOM	2126	N	THR	C1101	36.911	40.037	42.055	1.00	53.38
ATOM	2127	CA	THR	C1101	37.201	39.285	40.840	1.00	48.64
ATOM	2128	C	THR	C1101	36.746	37.835	41.057	1.00	46.24
ATOM	2129	O	THR	C1101	37.229	37.252	42.047	1.00	45.91
ATOM	2130	CB	THR	C1101	38.694	39.327	40.489	1.00	47.56
ATOM	2131	OG1	THR	C1101	39.019	40.606	39.939	1.00	46.44
ATOM	2132	CG2	THR	C1101	39.094	38.266	39.469	1.00	45.84
ATOM	2133	N	TYR	C1102	35.884	37.335	40.167	1.00	41.77
ATOM	2134	CA	TYR	C1102	35.366	35.978	40.426	1.00	40.39
ATOM	2135	C	TYR	C1102	36.129	34.910	39.691	1.00	40.66
ATOM	2136	O	TYR	C1102	36.056	33.736	40.095	1.00	42.76
ATOM	2137	CB	TYR	C1102	33.858	35.910	40.100	1.00	38.06
ATOM	2138	CG	TYR	C1102	33.074	36.622	41.174	1.00	39.42
ATOM	2139	CD1	TYR	C1102	32.812	37.986	41.085	1.00	40.49
ATOM	2140	CD2	TYR	C1102	32.609	35.932	42.296	1.00	40.20
ATOM	2141	CE1	TYR	C1102	32.107	38.642	42.061	1.00	41.47
ATOM	2142	CE2	TYR	C1102	31.904	36.580	43.294	1.00	41.62
ATOM	2143	CZ	TYR	C1102	31.672	37.936	43.168	1.00	42.72
ATOM	2144	OH	TYR	C1102	30.961	38.602	44.148	1.00	42.88
ATOM	2145	N	VAL	C1103	36.753	35.276	38.570	1.00	40.18
ATOM	2146	CA	VAL	C1103	37.580	34.400	37.772	1.00	38.79
ATOM	2147	C	VAL	C1103	38.963	35.061	37.561	1.00	40.96
ATOM	2148	O	VAL	C1103	39.070	36.083	36.864	1.00	41.22
ATOM	2149	CB	VAL	C1103	37.038	34.042	36.390	1.00	39.03
ATOM	2150	CG1	VAL	C1103	37.961	33.001	35.738	1.00	35.66
ATOM	2151	CG2	VAL	C1103	35.597	33.463	36.439	1.00	36.18
ATOM	2152	N	ASN	C1104	39.993	34.484	38.154	1.00	41.19
ATOM	2153	CA	ASN	C1104	41.366	34.972	38.131	1.00	43.68
ATOM	2154	C	ASN	C1104	42.006	34.745	36.765	1.00	42.39
ATOM	2155	O	ASN	C1104	42.161	33.569	36.390	1.00	46.58
ATOM	2156	CB	ASN	C1104	42.212	34.184	39.143	1.00	44.69
ATOM	2157	CG	ASN	C1104	43.661	34.686	39.140	1.00	49.43
ATOM	2158	OD1	ASN	C1104	44.630	33.918	38.841	1.00	49.14
ATOM	2159	ND2	ASN	C1104	43.739	35.989	39.460	1.00	47.59
ATOM	2160	N	THR	C1105	42.337	35.771	36.035	1.00	38.71

FIG. 5LL

ATOM	2161	CA	THR	C1105	42.937	35.664	34.723	1.00	38.30
ATOM	2162	C	THR	C1105	44.389	36.105	34.806	1.00	37.67
ATOM	2163	O	THR	C1105	44.998	36.087	33.725	1.00	39.99
ATOM	2164	CB	THR	C1105	42.272	36.465	33.585	1.00	36.40
ATOM	2165	OG1	THR	C1105	42.212	37.883	33.885	1.00	38.39
ATOM	2166	CG2	THR	C1105	40.875	35.906	33.439	1.00	35.66
ATOM	2167	N	THR	C1106	44.918	36.386	35.989	1.00	39.77
ATOM	2168	CA	THR	C1106	46.306	36.915	36.002	1.00	43.19
ATOM	2169	C	THR	C1106	47.368	35.852	36.199	1.00	44.10
ATOM	2170	O	THR	C1106	47.129	34.854	36.896	1.00	45.27
ATOM	2171	CB	THR	C1106	46.445	38.022	37.058	1.00	47.23
ATOM	2172	OG1	THR	C1106	46.210	37.460	38.369	1.00	52.99
ATOM	2173	CG2	THR	C1106	45.403	39.104	36.949	1.00	45.90
ATOM	2174	N	LEU	C1107	48.527	35.962	35.531	1.00	42.56
ATOM	2175	CA	LEU	C1107	49.593	34.961	35.679	1.00	44.02
ATOM	2176	C	LEU	C1107	50.420	35.168	36.946	1.00	46.86
ATOM	2177	O	LEU	C1107	50.888	36.295	37.127	1.00	49.56
ATOM	2178	CB	LEU	C1107	50.539	34.986	34.483	1.00	38.92
ATOM	2179	CG	LEU	C1107	49.970	34.778	33.106	1.00	37.89
ATOM	2180	CD1	LEU	C1107	51.073	34.991	32.082	1.00	39.13
ATOM	2181	CD2	LEU	C1107	49.400	33.350	32.925	1.00	34.26
ATOM	2182	N	TYR	C1108	50.605	34.176	37.803	1.00	49.68
ATOM	2183	CA	TYR	C1108	51.362	34.337	39.032	1.00	53.06
ATOM	2184	C	TYR	C1108	52.666	33.527	38.953	1.00	51.34
ATOM	2185	O	TYR	C1108	53.677	34.091	38.558	1.00	52.57
ATOM	2186	CB	TYR	C1108	50.645	33.861	40.328	1.00	54.61
ATOM	2187	CG	TYR	C1108	49.538	34.857	40.622	1.00	56.02
ATOM	2188	CD1	TYR	C1108	48.208	34.511	40.387	1.00	56.47
ATOM	2189	CD2	TYR	C1108	49.864	36.137	41.055	1.00	56.41
ATOM	2190	CE1	TYR	C1108	47.207	35.441	40.597	1.00	56.50
ATOM	2191	CE2	TYR	C1108	48.864	37.072	41.271	1.00	57.46
ATOM	2192	CZ	TYR	C1108	47.544	36.698	41.044	1.00	57.18
ATOM	2193	OH	TYR	C1108	46.577	37.639	41.267	1.00	58.64
ATOM	2194	N	GLU	C1109	52.585	32.293	39.382	1.00	50.07
ATOM	2195	CA	GLU	C1109	53.718	31.412	39.346	1.00	50.65
ATOM	2196	C	GLU	C1109	53.548	30.323	38.275	1.00	48.97
ATOM	2197	O	GLU	C1109	54.587	29.965	37.719	1.00	47.87
ATOM	2198	CB	GLU	C1109	53.958	30.616	40.626	1.00	53.87
ATOM	2199	CG	GLU	C1109	53.835	31.284	41.965	1.00	58.53
ATOM	2200	CD	GLU	C1109	54.896	32.352	42.202	1.00	60.45
ATOM	2201	OE1	GLU	C1109	56.092	31.991	42.113	1.00	61.68
ATOM	2202	OE2	GLU	C1109	54.482	33.514	42.480	1.00	61.69
ATOM	2203	N	LYS	C1110	52.345	29.727	38.224	1.00	47.13
ATOM	2204	CA	LYS	C1110	52.186	28.577	37.324	1.00	45.74
ATOM	2205	C	LYS	C1110	50.816	28.638	36.645	1.00	42.35
ATOM	2206	O	LYS	C1110	49.924	29.188	37.270	1.00	41.09
ATOM	2207	CB	LYS	C1110	52.400	27.320	38.151	1.00	48.67
ATOM	2208	CG	LYS	C1110	52.564	26.005	37.440	1.00	53.26
ATOM	2209	CD	LYS	C1110	53.174	24.877	38.287	1.00	56.04
ATOM	2210	CE	LYS	C1110	54.685	25.087	38.489	1.00	58.45
ATOM	2211	NZ	LYS	C1110	55.447	23.870	38.929	1.00	58.97
ATOM	2212	N	PHE	C1111	50.666	28.295	35.359	1.00	37.18
ATOM	2213	CA	PHE	C1111	49.325	28.434	34.823	1.00	36.07
ATOM	2214	C	PHE	C1111	49.163	27.464	33.658	1.00	33.65
ATOM	2215	O	PHE	C1111	49.926	27.605	32.736	1.00	31.39
ATOM	2216	CB	PHE	C1111	48.962	29.880	34.438	1.00	36.60
ATOM	2217	CG	PHE	C1111	47.531	30.157	34.143	1.00	37.58

FIG. 5MM

ATOM	2218	CD1	PHE	C1111	46.754	30.911	35.026	1.00	40.75
ATOM	2219	CD2	PHE	C1111	46.914	29.636	33.009	1.00	37.53
ATOM	2220	CE1	PHE	C1111	45.395	31.140	34.795	1.00	40.10
ATOM	2221	CE2	PHE	C1111	45.562	29.887	32.758	1.00	37.72
ATOM	2222	CZ	PHE	C1111	44.824	30.635	33.643	1.00	38.68
ATOM	2223	N	THR	C1112	48.115	26.664	33.719	1.00	28.79
ATOM	2224	CA	THR	C1112	47.688	25.828	32.634	1.00	31.45
ATOM	2225	C	THR	C1112	46.183	26.063	32.377	1.00	30.94
ATOM	2226	O	THR	C1112	45.468	26.129	33.377	1.00	29.01
ATOM	2227	CB	THR	C1112	47.744	24.317	33.099	1.00	32.34
ATOM	2228	OG1	THR	C1112	49.026	24.124	33.723	1.00	35.99
ATOM	2229	CG2	THR	C1112	47.738	23.401	31.909	1.00	32.22
ATOM	2230	N	TYR	C1113	45.708	26.099	31.158	1.00	28.73
ATOM	2231	CA	TYR	C1113	44.309	26.076	30.840	1.00	28.29
ATOM	2232	C	TYR	C1113	43.709	24.640	30.942	1.00	31.34
ATOM	2233	O	TYR	C1113	44.388	23.615	30.928	1.00	25.50
ATOM	2234	CB	TYR	C1113	44.203	26.353	29.330	1.00	27.79
ATOM	2235	CG	TYR	C1113	44.656	27.778	29.016	1.00	29.11
ATOM	2236	CD1	TYR	C1113	45.753	27.954	28.181	1.00	30.15
ATOM	2237	CD2	TYR	C1113	44.032	28.897	29.544	1.00	27.99
ATOM	2238	CE1	TYR	C1113	46.199	29.241	27.868	1.00	31.57
ATOM	2239	CE2	TYR	C1113	44.460	30.198	29.201	1.00	30.17
ATOM	2240	CZ	TYR	C1113	45.571	30.354	28.371	1.00	30.26
ATOM	2241	OH	TYR	C1113	46.068	31.611	28.045	1.00	30.20
ATOM	2242	N	ALA	C1114	42.398	24.636	31.120	1.00	29.12
ATOM	2243	CA	ALA	C1114	41.638	23.395	31.035	1.00	30.29
ATOM	2244	C	ALA	C1114	41.882	22.872	29.625	1.00	30.26
ATOM	2245	O	ALA	C1114	41.791	23.661	28.680	1.00	30.70
ATOM	2246	CB	ALA	C1114	40.127	23.678	31.199	1.00	30.91
ATOM	2247	N	GLY	C1115	42.135	21.544	29.515	1.00	28.43
ATOM	2248	CA	GLY	C1115	42.371	21.045	28.199	1.00	30.36
ATOM	2249	C	GLY	C1115	41.138	20.933	27.334	1.00	34.03
ATOM	2250	O	GLY	C1115	39.913	20.801	27.653	1.00	35.50
ATOM	2251	N	ILE	C1116	41.445	21.017	26.046	1.00	35.79
ATOM	2252	CA	ILE	C1116	40.554	20.877	24.918	1.00	41.16
ATOM	2253	C	ILE	C1116	40.987	19.601	24.199	1.00	48.93
ATOM	2254	CB	ILE	C1116	40.660	21.990	23.877	1.00	40.53
ATOM	2255	CG1	ILE	C1116	40.332	23.381	24.419	1.00	39.34
ATOM	2256	CG2	ILE	C1116	39.797	21.709	22.629	1.00	40.56
ATOM	2257	CD1	ILE	C1116	40.844	24.462	23.474	1.00	39.48
ATOM	2258	N	ASP	C1117	40.096	18.690	23.816	1.00	56.34
ATOM	2259	CA	ASP	C1117	40.671	17.809	22.759	1.00	64.41
ATOM	2260	C	ASP	C1117	39.582	17.226	21.862	1.00	67.05
ATOM	2261	O	ASP	C1117	38.632	16.639	22.384	1.00	66.11
ATOM	2262	CB	ASP	C1117	41.552	16.679	23.243	1.00	66.12
ATOM	2263	CG	ASP	C1117	42.980	17.054	23.608	1.00	68.11
ATOM	2264	OD1	ASP	C1117	43.730	17.676	22.830	1.00	69.52
ATOM	2265	OD2	ASP	C1117	43.216	16.706	24.787	1.00	68.31
ATOM	2266	N	CYS	C1118	39.775	17.421	20.548	1.00	71.27
ATOM	2267	CA	CYS	C1118	38.800	16.948	19.563	1.00	75.06
ATOM	2268	C	CYS	C1118	39.057	17.522	18.165	1.00	77.90
ATOM	2269	CB	CYS	C1118	37.387	17.351	19.997	1.00	74.91
ATOM	2270	N	SER	C1119	38.094	17.334	17.244	1.00	81.20
ATOM	2271	CA	SER	C1119	38.055	17.960	15.924	1.00	83.28
ATOM	2272	C	SER	C1119	37.335	17.232	14.787	1.00	84.56
ATOM	2273	O	SER	C1119	37.930	16.898	13.740	1.00	85.44
ATOM	2274	CB	SER	C1119	39.493	18.300	15.476	1.00	83.21

FIG. 5NN

```
ATOM   2275  N   ALA C1120      36.028  16.990  14.863  1.00 85.16
ATOM   2276  CA  ALA C1120      35.171  16.384  13.874  1.00 84.89
ATOM   2277  C   ALA C1120      34.722  14.957  14.213  1.00 85.19
ATOM   2278  O   ALA C1120      33.876  14.494  13.396  1.00 85.38
ATOM   2279  CB  ALA C1120      35.714  16.345  12.447  1.00 84.84
TER
HETATM 2280  C1  IN3 D   1      27.737  34.907  12.224  1.00 40.84
HETATM 2281  N2  IN3 D   1      28.220  33.661  12.185  1.00 40.67
HETATM 2282  C3  IN3 D   1      27.362  32.629  12.233  1.00 40.61
HETATM 2283  C4  IN3 D   1      25.970  32.787  12.323  1.00 41.94
HETATM 2284  C5  IN3 D   1      25.529  34.130  12.362  1.00 41.03
HETATM 2285  N6  IN3 D   1      26.428  35.160  12.315  1.00 40.65
HETATM 2287  N8  IN3 D   1      27.727  31.299  12.203  1.00 42.23
HETATM 2288  C9  IN3 D   1      26.517  30.664  12.312  1.00 42.50
HETATM 2289  C10 IN3 D   1      25.373  31.506  12.348  1.00 44.61
HETATM 2291  N12 IN3 D   1      24.221  34.490  12.467  1.00 43.99
HETATM 2292  C13 IN3 D   1      23.982  30.977  12.436  1.00 47.57
HETATM 2293  C14 IN3 D   1      29.096  30.727  12.190  1.00 42.52
HETATM 2294  C15 IN3 D   1      22.960  31.497  13.194  1.00 50.46
HETATM 2295  C16 IN3 D   1      21.667  30.935  13.250  1.00 51.20
HETATM 2296  C17 IN3 D   1      21.337  29.804  12.531  1.00 51.31
HETATM 2297  C18 IN3 D   1      22.357  29.258  11.751  1.00 51.58
HETATM 2298  C19 IN3 D   1      23.637  29.839  11.712  1.00 51.00
HETATM 2302  N23 IN3 D   1      20.099  29.245  12.581  1.00 52.79
HETATM 2303  S24 IN3 D   1      19.137  29.209  13.847  1.00 53.21
HETATM 2304  O25 IN3 D   1      19.809  29.557  15.058  1.00 54.86
HETATM 2305  O26 IN3 D   1      18.402  27.997  13.940  1.00 52.02
HETATM 2306  C27 IN3 D   1      17.984  30.563  13.554  1.00 59.14
HETATM 2307  C28 IN3 D   1      17.058  30.565  12.515  1.00 62.44
HETATM 2308  C29 IN3 D   1      16.171  31.631  12.344  1.00 63.41
HETATM 2309  C30 IN3 D   1      16.219  32.721  13.201  1.00 61.99
HETATM 2310  C31 IN3 D   1      17.146  32.728  14.233  1.00 61.19
HETATM 2311  C32 IN3 D   1      18.012  31.655  14.412  1.00 59.69
HETATM 2312 CL33 IN3 D   1      17.000  29.190  11.437  1.00 72.20
HETATM 2313 CL34 IN3 D   1      14.971  31.634  11.070  1.00 66.32
HETATM 2317  F38 IN3 D   1      22.188  28.164  10.970  1.00 50.23
HETATM 2318  C39 IN3 D   1      29.429  30.465  13.689  1.00 41.55
HETATM 2319  C40 IN3 D   1      30.719  29.713  13.975  1.00 41.76
HETATM 2320  C41 IN3 D   1      30.922  28.491  13.060  1.00 42.34
HETATM 2321  C42 IN3 D   1      30.611  28.800  11.579  1.00 44.10
HETATM 2322  C43 IN3 D   1      29.231  29.447  11.376  1.00 43.74
HETATM 2331  C52 IN3 D   1      32.457  27.054  14.408  1.00 40.98
HETATM 2332  C53 IN3 D   1      33.702  26.161  14.218  1.00 39.93
HETATM 2333  N54 IN3 D   1      34.865  27.024  14.047  1.00 40.92
HETATM 2334  C55 IN3 D   1      34.719  27.865  12.858  1.00 41.55
HETATM 2335  C56 IN3 D   1      33.437  28.707  12.946  1.00 41.49
HETATM 2336  N57 IN3 D   1      32.249  27.891  13.211  1.00 41.23
HETATM 2346  C67 IN3 D   1      36.230  26.430  14.126  1.00 38.95
TER
ATOM   2355  O   HOH W   1      31.108  33.861  12.284  1.00 32.88
ATOM   2356  O   HOH W   2      26.872  17.118  31.780  1.00 27.53
ATOM   2357  O   HOH W   3      33.552  31.769  15.218  1.00 24.69
ATOM   2358  O   HOH W   4      47.567  25.314  28.603  1.00 31.73
ATOM   2359  O   HOH W   5       2.429  17.063  30.925  1.00 30.32
ATOM   2360  O   HOH W   7      33.908  23.176  25.246  1.00 32.79
ATOM   2361  O   HOH W   8      16.942  20.674  27.837  1.00 29.27
ATOM   2362  O   HOH W   9      41.194  27.270  31.243  1.00 27.50
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FIG. 50O

ATOM	2363	O	HOH	W	10	36.797	18.417	32.828	1.00	30.03
ATOM	2364	O	HOH	W	11	28.851	18.044	36.031	1.00	31.03
ATOM	2365	O	HOH	W	12	15.509	25.207	20.371	1.00	36.36
ATOM	2366	O	HOH	W	13	9.416	22.554	31.309	1.00	34.74
ATOM	2367	O	HOH	W	14	24.583	41.060	16.124	1.00	44.69
ATOM	2368	O	HOH	W	15	7.357	41.316	15.797	1.00	65.05
ATOM	2369	O	HOH	W	16	40.089	39.018	35.286	1.00	43.58
ATOM	2370	O	HOH	W	17	42.573	39.050	31.498	1.00	33.36
ATOM	2371	O	HOH	W	18	18.935	40.500	18.279	1.00	34.03
ATOM	2372	O	HOH	W	19	13.481	27.068	41.482	1.00	45.27
ATOM	2373	O	HOH	W	20	19.798	23.284	27.046	1.00	32.39
ATOM	2374	O	HOH	W	22	13.750	26.546	29.238	1.00	33.61
ATOM	2375	O	HOH	W	23	15.599	37.531	37.224	1.00	41.73
ATOM	2376	O	HOH	W	24	45.162	20.392	30.028	1.00	51.51
ATOM	2377	O	HOH	W	25	33.164	26.427	17.812	1.00	30.96
ATOM	2378	O	HOH	W	27	25.096	40.967	30.617	1.00	31.07
ATOM	2379	O	HOH	W	28	44.306	23.553	33.708	1.00	44.45
ATOM	2380	O	HOH	W	29	14.071	17.249	33.601	1.00	32.43
ATOM	2381	O	HOH	W	30	30.157	24.039	23.053	1.00	31.23
ATOM	2382	O	HOH	W	31	21.111	43.623	15.597	1.00	74.93
ATOM	2383	O	HOH	W	33	19.327	17.632	28.859	1.00	33.09
ATOM	2384	O	HOH	W	34	13.241	23.665	39.267	1.00	41.89
ATOM	2385	O	HOH	W	35	31.519	44.776	18.549	1.00	43.36
ATOM	2386	O	HOH	W	36	34.470	39.819	38.307	1.00	52.30
ATOM	2387	O	HOH	W	37	19.740	20.765	27.651	1.00	65.54
ATOM	2388	O	HOH	W	38	44.917	36.546	20.426	1.00	59.90
ATOM	2389	O	HOH	W	40	17.011	9.839	35.866	1.00	47.22
ATOM	2390	O	HOH	W	41	38.945	20.370	30.087	1.00	25.50
ATOM	2391	O	HOH	W	43	46.179	22.872	28.085	1.00	39.76
ATOM	2392	O	HOH	W	44	33.414	46.660	18.569	1.00	52.18
ATOM	2393	O	HOH	W	45	25.781	19.393	41.795	1.00	39.77
ATOM	2394	O	HOH	W	46	25.879	14.880	30.825	1.00	26.83
ATOM	2395	O	HOH	W	47	12.674	31.920	35.287	1.00	41.22
ATOM	2396	O	HOH	W	48	36.038	20.519	22.613	1.00	40.75
ATOM	2397	O	HOH	W	49	9.232	35.876	28.692	1.00	40.36
ATOM	2398	O	HOH	W	50	36.218	20.561	20.320	1.00	41.55
ATOM	2399	O	HOH	W	54	27.796	43.597	11.505	1.00	56.18
ATOM	2400	O	HOH	W	56	43.257	28.114	21.417	1.00	40.56
ATOM	2401	O	HOH	W	57	42.324	44.229	29.443	1.00	56.40
ATOM	2402	O	HOH	W	58	31.439	22.023	21.413	1.00	32.43
ATOM	2403	O	HOH	W	59	49.313	32.007	37.867	1.00	46.71
ATOM	2404	O	HOH	W	60	14.875	35.132	15.522	1.00	39.98
ATOM	2405	O	HOH	W	62	20.722	5.005	29.475	1.00	39.73
ATOM	2406	O	HOH	W	63	45.974	43.256	29.290	1.00	41.18
ATOM	2407	O	HOH	W	64	42.241	38.248	37.028	1.00	43.70
ATOM	2408	O	HOH	W	65	32.550	42.002	39.832	1.00	36.99
ATOM	2409	O	HOH	W	67	39.110	46.531	21.311	1.00	37.71
ATOM	2410	O	HOH	W	68	24.108	20.905	21.953	1.00	53.77
ATOM	2411	O	HOH	W	69	1.460	21.994	31.199	1.00	37.30
ATOM	2412	O	HOH	W	70	49.466	21.211	34.770	1.00	51.34
ATOM	2413	O	HOH	W	71	36.003	21.023	42.825	1.00	40.91
ATOM	2414	O	HOH	W	73	22.188	25.684	4.901	1.00	54.10
ATOM	2415	O	HOH	W	74	39.079	46.157	42.492	1.00	62.53
ATOM	2416	O	HOH	W	75	40.067	30.895	33.482	1.00	47.79
ATOM	2417	O	HOH	W	76	46.668	20.370	34.397	1.00	41.58
ATOM	2418	O	HOH	W	78	11.682	32.018	39.657	1.00	44.53
ATOM	2419	O	HOH	W	79	20.567	30.929	42.014	1.00	56.17

FIG. 5PP

ATOM	2420	O	HOH	W	80	22.313	16.019	43.949	1.00	47.96
ATOM	2421	O	HOH	W	83	33.379	32.767	48.175	1.00	44.70
ATOM	2422	O	HOH	W	84	28.448	47.110	11.329	1.00	72.32
ATOM	2423	O	HOH	W	85	11.988	40.527	14.366	1.00	57.96
ATOM	2424	O	HOH	W	86	11.100	37.338	30.951	1.00	55.75
ATOM	2425	O	HOH	W	87	32.424	25.662	10.927	1.00	60.85
ATOM	2426	O	HOH	W	88	40.553	21.024	36.981	1.00	56.71
ATOM	2427	O	HOH	W	89	20.806	40.663	41.692	1.00	49.92
ATOM	2428	O	HOH	W	90	23.126	21.071	24.579	1.00	28.98
ATOM	2429	O	HOH	W	91	21.847	27.668	22.076	1.00	39.04
ATOM	2430	O	HOH	W	92	17.442	12.682	22.568	1.00	42.46
ATOM	2431	O	HOH	W	94	10.365	22.725	38.862	1.00	42.24
ATOM	2432	O	HOH	W	96	12.915	13.110	35.504	1.00	43.57
ATOM	2433	O	HOH	W	97	11.437	18.561	35.709	1.00	49.64
ATOM	2434	O	HOH	W	98	18.202	17.009	21.807	1.00	60.40
ATOM	2435	O	HOH	W	99	13.090	22.057	22.029	1.00	44.65
ATOM	2436	O	HOH	W	100	13.782	3.003	30.101	1.00	45.94
ATOM	2437	O	HOH	W	101	37.114	30.510	14.091	1.00	54.40
ATOM	2438	O	HOH	W	102	39.281	19.995	32.505	1.00	38.67
ATOM	2439	O	HOH	W	103	19.163	41.538	33.907	1.00	49.16
ATOM	2440	O	HOH	W	105	8.161	24.650	30.444	1.00	38.87
ATOM	2441	O	HOH	W	106	19.044	34.146	43.247	1.00	36.17
ATOM	2442	O	HOH	W	107	52.411	29.944	20.957	1.00	47.78
ATOM	2443	O	HOH	W	109	40.926	37.945	21.207	1.00	57.61
ATOM	2444	O	HOH	W	110	23.910	22.805	45.525	1.00	56.43
ATOM	2445	O	HOH	W	111	23.876	43.384	19.810	1.00	29.77
ATOM	2446	O	HOH	W	112	6.751	36.672	21.579	1.00	62.88
ATOM	2447	O	HOH	W	113	43.463	27.806	35.372	1.00	49.32
ATOM	2448	O	HOH	W	114	33.230	32.283	12.794	1.00	37.37
ATOM	2449	O	HOH	W	115	39.120	18.996	40.839	1.00	82.49
ATOM	2450	O	HOH	W	116	17.786	13.772	37.357	1.00	49.91
ATOM	2451	O	HOH	W	117	20.655	9.465	38.822	1.00	43.82
ATOM	2452	O	HOH	W	118	7.544	39.794	24.678	1.00	56.43
ATOM	2453	O	HOH	W	119	34.363	21.476	9.358	1.00	64.39
ATOM	2454	O	HOH	W	120	14.923	37.925	31.147	1.00	51.98
ATOM	2455	O	HOH	W	121	14.386	25.644	36.407	1.00	47.28
ATOM	2456	O	HOH	W	122	33.578	21.114	23.402	1.00	36.98
ATOM	2457	O	HOH	W	123	42.616	19.765	31.993	1.00	46.67
ATOM	2458	O	HOH	W	124	0.324	31.122	29.775	1.00	85.67
ATOM	2459	O	HOH	W	125	44.223	21.073	33.792	1.00	58.84
ATOM	2460	O	HOH	W	126	13.220	29.507	33.957	1.00	42.26
ATOM	2461	O	HOH	W	127	24.661	6.250	44.308	1.00	53.58
ATOM	2462	O	HOH	W	130	37.555	26.025	18.301	1.00	50.21
ATOM	2463	O	HOH	W	131	29.409	15.521	23.790	1.00	37.37
ATOM	2464	O	HOH	W	134	37.198	41.960	35.518	1.00	40.19
ATOM	2465	O	HOH	W	135	38.741	36.516	21.186	1.00	31.33
ATOM	2466	O	HOH	W	136	20.039	45.048	11.998	1.00	67.09
ATOM	2467	O	HOH	W	137	44.865	39.383	33.992	1.00	42.87
ATOM	2468	O	HOH	W	138	47.499	41.543	34.693	1.00	41.95
ATOM	2469	O	HOH	W	139	14.470	39.588	29.214	1.00	39.88
ATOM	2470	O	HOH	W	140	25.148	21.128	18.186	1.00	55.16
ATOM	2471	O	HOH	W	141	19.506	9.850	24.839	1.00	56.90
ATOM	2472	O	HOH	W	142	39.082	7.569	29.845	1.00	50.85
ATOM	2473	O	HOH	W	143	37.915	8.580	37.497	1.00	73.18
ATOM	2474	O	HOH	W	144	37.234	11.075	36.059	1.00	55.17
ATOM	2475	O	HOH	W	145	18.909	16.767	43.975	1.00	45.07
ATOM	2476	O	HOH	W	146	53.564	36.062	20.842	1.00	35.39

FIG. 500

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ATOM   2477  O   HOH W 147      21.172  42.848  12.347  1.00 52.85
TER
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FIG. 5RR

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ATOM      1  N   VAL A 818      77.717  45.877   1.677  1.00100.00
ATOM      2  CA  VAL A 818      76.698  46.966   1.561  1.00100.00
ATOM      3  C   VAL A 818      75.278  46.411   1.674  1.00100.00
ATOM      4  O   VAL A 818      74.803  46.162   2.781  1.00100.00
ATOM      5  CB  VAL A 818      76.875  47.697   0.239  1.00 68.23
ATOM      9  N   LEU A 819      74.617  46.228   0.530  1.00100.00
ATOM     10  CA  LEU A 819      73.248  45.707   0.456  1.00100.00
ATOM     11  C   LEU A 819      72.629  45.997  -0.918  1.00100.00
ATOM     12  O   LEU A 819      71.622  46.689  -1.003  1.00100.00
ATOM     13  CB  LEU A 819      72.369  46.345   1.536  1.00100.00
ATOM     14  CG  LEU A 819      70.873  46.053   1.525  1.00100.00
ATOM     15  CD1 LEU A 819      70.592  44.975   2.511  1.00100.00
ATOM     16  CD2 LEU A 819      70.078  47.283   1.865  1.00100.00
ATOM     18  N   ASP A 820      73.234  45.474  -1.984  1.00100.00
ATOM     19  CA  ASP A 820      72.753  45.676  -3.359  1.00100.00
ATOM     20  C   ASP A 820      71.292  46.104  -3.464  1.00100.00
ATOM     21  O   ASP A 820      70.399  45.421  -2.983  1.00100.00
ATOM     22  CB  ASP A 820      72.969  44.396  -4.177  1.00 99.21
ATOM     23  CG  ASP A 820      71.872  44.160  -5.218  1.00 99.21
ATOM     24  OD1 ASP A 820      71.584  42.982  -5.509  1.00 99.21
ATOM     25  OD2 ASP A 820      71.303  45.140  -5.750  1.00 99.21
ATOM     27  N   TRP A 821      71.050  47.227  -4.126  1.00 93.11
ATOM     28  CA  TRP A 821      69.694  47.719  -4.268  1.00 93.11
ATOM     29  C   TRP A 821      68.716  46.617  -4.650  1.00 93.11
ATOM     30  O   TRP A 821      67.904  46.199  -3.849  1.00 93.11
ATOM     31  CB  TRP A 821      69.639  48.863  -5.283  1.00 97.87
ATOM     32  CG  TRP A 821      68.703  49.927  -4.847  1.00 97.87
ATOM     33  CD1 TRP A 821      68.605  50.452  -3.597  1.00 97.87
ATOM     34  CD2 TRP A 821      67.667  50.542  -5.622  1.00 97.87
ATOM     35  NE1 TRP A 821      67.567  51.352  -3.537  1.00 97.87
ATOM     36  CE2 TRP A 821      66.974  51.429  -4.766  1.00 97.87
ATOM     37  CE3 TRP A 821      67.255  50.429  -6.949  1.00 97.87
ATOM     38  CZ2 TRP A 821      65.897  52.197  -5.193  1.00 97.87
ATOM     39  CZ3 TRP A 821      66.180  51.192  -7.374  1.00 97.87
ATOM     40  CH2 TRP A 821      65.512  52.065  -6.496  1.00 97.87
ATOM     43  N   ASN A 822      68.798  46.140  -5.896  1.00100.00
ATOM     44  CA  ASN A 822      67.901  45.077  -6.364  1.00100.00
ATOM     45  C   ASN A 822      67.686  43.985  -5.314  1.00100.00
ATOM     46  O   ASN A 822      66.545  43.614  -5.030  1.00100.00
ATOM     47  CB  ASN A 822      68.462  44.410  -7.624  1.00 56.29
ATOM     48  CG  ASN A 822      68.707  42.917  -7.427  1.00 56.29
ATOM     49  OD1 ASN A 822      69.755  42.499  -6.902  1.00 56.29
ATOM     50  ND2 ASN A 822      67.739  42.114  -7.837  1.00 56.29
ATOM     54  N   ASP A 823      68.799  43.469  -4.776  1.00 99.96
ATOM     55  CA  ASP A 823      68.825  42.413  -3.756  1.00 99.96
ATOM     56  C   ASP A 823      67.823  42.654  -2.650  1.00 99.96
ATOM     57  O   ASP A 823      67.545  41.765  -1.846  1.00 99.96
ATOM     58  CB  ASP A 823      70.218  42.308  -3.153  1.00100.00
ATOM     60  N   ILE A 824      67.303  43.875  -2.605  1.00 80.08
ATOM     61  CA  ILE A 824      66.315  44.270  -1.616  1.00 80.08
ATOM     62  C   ILE A 824      64.958  44.392  -2.274  1.00 80.08
ATOM     63  O   ILE A 824      64.703  45.359  -2.973  1.00 80.08
ATOM     64  CB  ILE A 824      66.651  45.641  -0.992  1.00100.00
ATOM     65  CG1 ILE A 824      67.806  45.506   0.009  1.00100.00
ATOM     66  CG2 ILE A 824      65.417  46.206  -0.307  1.00100.00
ATOM     67  CD1 ILE A 824      69.048  44.906  -0.577  1.00100.00
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FIG. 6A

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ATOM     69  N   LYS A 825      64.098  43.404  -2.036  1.00 99.67
ATOM     70  CA  LYS A 825      62.735  43.391  -2.580  1.00 99.67
ATOM     71  C   LYS A 825      61.938  44.544  -1.938  1.00 99.67
ATOM     72  O   LYS A 825      61.130  44.334  -1.027  1.00 99.67
ATOM     73  CB  LYS A 825      62.056  42.021  -2.286  1.00 63.59
ATOM     75  N   PHE A 826      62.171  45.762  -2.420  1.00 69.32
ATOM     76  CA  PHE A 826      61.502  46.933  -1.875  1.00 69.32
ATOM     77  C   PHE A 826      59.977  46.823  -1.994  1.00 69.32
ATOM     78  O   PHE A 826      59.500  45.922  -2.684  1.00 69.32
ATOM     79  CB  PHE A 826      62.060  48.158  -2.587  1.00 99.11
ATOM     80  CG  PHE A 826      63.558  48.351  -2.376  1.00 99.11
ATOM     81  CD1 PHE A 826      64.470  47.961  -3.343  1.00 99.11
ATOM     82  CD2 PHE A 826      64.045  48.959  -1.215  1.00 99.11
ATOM     83  CE1 PHE A 826      65.839  48.178  -3.157  1.00 99.11
ATOM     84  CE2 PHE A 826      65.418  49.179  -1.027  1.00 99.11
ATOM     85  CZ  PHE A 826      66.307  48.791  -1.995  1.00 99.11
ATOM     87  N   GLN A 827      59.222  47.691  -1.307  1.00 70.60
ATOM     88  CA  GLN A 827      57.728  47.659  -1.347  1.00 70.60
ATOM     89  C   GLN A 827      57.010  49.023  -1.173  1.00 70.60
ATOM     90  O   GLN A 827      57.401  49.946  -1.874  1.00 70.60
ATOM     91  CB  GLN A 827      57.178  46.624  -0.337  1.00100.00
ATOM     92  CG  GLN A 827      57.627  45.151  -0.598  1.00100.00
ATOM     93  CD  GLN A 827      56.797  44.413  -1.665  1.00100.00
ATOM     94  OE1 GLN A 827      55.642  44.036  -1.433  1.00100.00
ATOM     95  NE2 GLN A 827      57.396  44.196  -2.831  1.00100.00
ATOM     99  N   ASP A 828      56.000  49.149  -0.278  1.00 99.97
ATOM    100  CA  ASP A 828      55.218  50.418  -0.055  1.00 99.97
ATOM    101  C   ASP A 828      55.490  51.355   1.163  1.00 99.97
ATOM    102  O   ASP A 828      56.284  51.045   2.038  1.00 99.97
ATOM    103  CB  ASP A 828      53.723  50.128   0.010  1.00100.00
ATOM    104  CG  ASP A 828      53.034  50.839   1.214  1.00100.00
ATOM    105  OD1 ASP A 828      52.702  52.037   1.109  1.00100.00
ATOM    106  OD2 ASP A 828      52.834  50.215   2.280  1.00100.00
ATOM    108  N   VAL A 829      54.787  52.494   1.212  1.00100.00
ATOM    109  CA  VAL A 829      54.900  53.488   2.295  1.00100.00
ATOM    110  C   VAL A 829      54.384  53.014   3.639  1.00100.00
ATOM    111  O   VAL A 829      53.683  52.012   3.703  1.00100.00
ATOM    112  CB  VAL A 829      54.162  54.786   1.912  1.00100.00
ATOM    114  N   ILE A 830      54.726  53.770   4.695  1.00 76.50
ATOM    115  CA  ILE A 830      54.342  53.500   6.102  1.00 76.50
ATOM    116  C   ILE A 830      53.685  54.717   6.782  1.00 76.50
ATOM    117  O   ILE A 830      52.464  54.830   6.808  1.00 76.50
ATOM    118  CB  ILE A 830      55.571  53.069   6.979  1.00 83.02
ATOM    119  CG1 ILE A 830      55.888  51.607   6.755  1.00 83.02
ATOM    120  CG2 ILE A 830      55.269  53.185   8.437  1.00 83.02
ATOM    121  CD1 ILE A 830      57.118  51.163   7.437  1.00 83.02
ATOM    123  N   GLY A 831      54.492  55.626   7.327  1.00100.00
ATOM    124  CA  GLY A 831      53.930  56.779   8.009  1.00100.00
ATOM    125  C   GLY A 831      54.664  58.090   7.811  1.00100.00
ATOM    126  O   GLY A 831      54.659  58.963   8.677  1.00100.00
ATOM    128  N   GLU A 832      55.301  58.216   6.660  1.00 46.31
ATOM    129  CA  GLU A 832      56.045  59.418   6.271  1.00 46.31
ATOM    130  C   GLU A 832      57.586  59.215   6.265  1.00 46.31
ATOM    131  O   GLU A 832      58.101  58.149   5.892  1.00 46.31
ATOM    132  CB  GLU A 832      55.668  60.618   7.158  1.00100.00
ATOM    133  CG  GLU A 832      54.587  61.531   6.557  1.00100.00
ATOM    134  CD  GLU A 832      54.197  62.702   7.473  1.00100.00
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FIG. 6B

ATOM	185	OE1	GLU	A	832	52.980	62.942	7.660	1.00100.00
ATOM	186	OE2	GLU	A	832	55.107	63.387	8.002	1.00100.00
ATOM	138	N	GLY	A	833	58.330	60.239	6.650	1.00100.00
ATOM	139	CA	GLY	A	833	59.762	60.092	6.672	1.00100.00
ATOM	140	C	GLY	A	833	60.311	61.410	7.090	1.00100.00
ATOM	141	O	GLY	A	833	60.675	61.601	8.251	1.00100.00
ATOM	143	N	ASN	A	834	60.339	62.327	6.130	1.00 87.28
ATOM	144	CA	ASN	A	834	60.829	63.680	6.360	1.00 87.28
ATOM	145	C	ASN	A	834	62.306	63.520	6.639	1.00 87.28
ATOM	146	O	ASN	A	834	62.684	62.859	7.613	1.00 87.28
ATOM	147	CB	ASN	A	834	60.114	64.306	7.570	1.00100.00
ATOM	148	CG	ASN	A	834	60.641	65.685	7.932	1.00100.00
ATOM	149	OD1	ASN	A	834	61.822	65.865	8.248	1.00100.00
ATOM	150	ND2	ASN	A	834	59.751	66.671	7.903	1.00100.00
ATOM	154	N	PHE	A	835	63.131	64.125	5.782	1.00 68.16
ATOM	155	CA	PHE	A	835	64.561	64.036	5.925	1.00 68.16
ATOM	156	C	PHE	A	835	64.700	62.693	6.578	1.00 68.16
ATOM	157	O	PHE	A	835	65.138	62.586	7.733	1.00 68.16
ATOM	158	CB	PHE	A	835	65.073	65.139	6.840	1.00 80.78
ATOM	159	CG	PHE	A	835	65.317	66.447	6.135	1.00 80.78
ATOM	160	CD1	PHE	A	835	64.950	67.651	6.733	1.00 80.78
ATOM	161	CD2	PHE	A	835	65.931	66.475	4.877	1.00 80.78
ATOM	162	CE1	PHE	A	835	65.190	68.856	6.097	1.00 80.78
ATOM	163	CE2	PHE	A	835	66.178	67.689	4.226	1.00 80.78
ATOM	164	CZ	PHE	A	835	65.805	68.881	4.838	1.00 80.78
ATOM	166	N	GLY	A	836	64.226	61.691	5.832	1.00100.00
ATOM	167	CA	GLY	A	836	64.252	60.304	6.257	1.00100.00
ATOM	168	C	GLY	A	836	62.962	59.578	5.914	1.00100.00
ATOM	169	O	GLY	A	836	62.314	59.012	6.792	1.00100.00
ATOM	171	N	GLN	A	837	62.599	59.565	4.636	1.00 88.37
ATOM	172	CA	GLN	A	837	61.356	58.915	4.214	1.00 88.37
ATOM	173	C	GLN	A	837	61.114	57.472	4.701	1.00 88.37
ATOM	174	O	GLN	A	837	61.739	56.544	4.186	1.00 88.37
ATOM	175	CB	GLN	A	837	61.206	58.983	2.666	1.00 70.59
ATOM	176	CG	GLN	A	837	62.424	58.531	1.876	1.00 70.59
ATOM	177	CD	GLN	A	837	62.484	59.097	0.437	1.00 70.59
ATOM	178	OE1	GLN	A	837	63.560	59.517	-0.041	1.00 70.59
ATOM	179	NE2	GLN	A	837	61.327	59.088	-0.263	1.00 70.59
ATOM	183	N	VAL	A	838	60.211	57.302	5.687	1.00 63.61
ATOM	184	CA	VAL	A	838	59.835	55.959	6.213	1.00 63.61
ATOM	185	C	VAL	A	838	58.710	55.222	5.481	1.00 63.61
ATOM	186	O	VAL	A	838	57.525	55.380	5.807	1.00 63.61
ATOM	187	CB	VAL	A	838	59.384	55.939	7.692	1.00 61.77
ATOM	188	CG1	VAL	A	838	60.243	54.967	8.446	1.00 61.77
ATOM	189	CG2	VAL	A	838	59.418	57.290	8.292	1.00 61.77
ATOM	191	N	LEU	A	839	59.114	54.397	4.520	1.00100.00
ATOM	192	CA	LEU	A	839	58.201	53.584	3.738	1.00100.00
ATOM	193	C	LEU	A	839	58.399	52.107	4.098	1.00100.00
ATOM	194	O	LEU	A	839	59.473	51.694	4.507	1.00100.00
ATOM	195	CB	LEU	A	839	58.464	53.783	2.244	1.00100.00
ATOM	196	CG	LEU	A	839	58.836	55.168	1.719	1.00100.00
ATOM	197	CD1	LEU	A	839	58.069	56.233	2.461	1.00100.00
ATOM	198	CD2	LEU	A	839	60.323	55.367	1.853	1.00100.00
ATOM	200	N	LYS	A	840	57.352	51.315	3.969	1.00 58.16
ATOM	201	CA	LYS	A	840	57.459	49.901	4.259	1.00 58.16
ATOM	202	C	LYS	A	840	58.091	49.174	3.081	1.00 58.16
ATOM	203	O	LYS	A	840	57.837	49.497	1.943	1.00 58.16

FIG. 6C

ATOM	204	CB	LYS	A	840	56.071	49.313	4.549	1.00	67.71
ATOM	205	CG	LYS	A	840	56.075	47.809	4.810	1.00	67.71
ATOM	206	CD	LYS	A	840	55.274	47.391	6.047	1.00	67.71
ATOM	207	CE	LYS	A	840	55.467	45.926	6.360	1.00	67.71
ATOM	208	NZ	LYS	A	840	56.848	45.463	6.017	1.00	67.71
ATOM	213	N	ALA	A	841	58.916	48.176	3.344	1.00	99.75
ATOM	214	CA	ALA	A	841	59.514	47.452	2.241	1.00	99.75
ATOM	215	C	ALA	A	841	59.845	46.037	2.620	1.00	99.75
ATOM	216	O	ALA	A	841	59.830	45.684	3.796	1.00	99.75
ATOM	217	CB	ALA	A	841	60.748	48.152	1.771	1.00	78.22
ATOM	219	N	ARG	A	842	60.143	45.231	1.605	1.00	100.00
ATOM	220	CA	ARG	A	842	60.499	43.832	1.798	1.00	100.00
ATOM	221	C	ARG	A	842	61.972	43.576	1.429	1.00	100.00
ATOM	222	O	ARG	A	842	62.288	43.082	0.352	1.00	100.00
ATOM	223	CB	ARG	A	842	59.574	42.951	0.973	1.00	100.00
ATOM	225	N	ILE	A	843	62.868	43.919	2.348	1.00	100.00
ATOM	226	CA	ILE	A	843	64.301	43.743	2.148	1.00	100.00
ATOM	227	C	ILE	A	843	64.642	42.262	2.174	1.00	100.00
ATOM	228	O	ILE	A	843	63.952	41.488	2.844	1.00	100.00
ATOM	229	CB	ILE	A	843	65.094	44.489	3.263	1.00	99.77
ATOM	230	CG1	ILE	A	843	65.193	45.960	2.907	1.00	99.77
ATOM	231	CG2	ILE	A	843	66.487	43.937	3.421	1.00	99.77
ATOM	232	CD1	ILE	A	843	63.857	46.576	2.554	1.00	99.77
ATOM	234	N	LYS	A	844	65.691	41.882	1.435	1.00	77.20
ATOM	235	CA	LYS	A	844	66.176	40.501	1.379	1.00	77.20
ATOM	236	C	LYS	A	844	67.635	40.390	1.854	1.00	77.20
ATOM	237	O	LYS	A	844	68.499	41.059	1.313	1.00	77.20
ATOM	238	CB	LYS	A	844	66.063	39.973	-0.045	1.00	63.87
ATOM	240	N	LYS	A	845	67.921	39.570	2.859	1.00	93.93
ATOM	241	CA	LYS	A	845	69.313	39.419	3.302	1.00	93.93
ATOM	242	C	LYS	A	845	69.979	38.431	2.382	1.00	93.93
ATOM	243	O	LYS	A	845	69.341	37.931	1.453	1.00	93.93
ATOM	244	CB	LYS	A	845	69.391	38.854	4.684	1.00	20.96
ATOM	246	N	ASP	A	846	71.258	38.140	2.631	1.00	72.18
ATOM	247	CA	ASP	A	846	71.912	37.136	1.815	1.00	72.18
ATOM	248	C	ASP	A	846	70.882	36.018	2.059	1.00	72.18
ATOM	249	O	ASP	A	846	70.861	35.389	3.129	1.00	72.18
ATOM	250	CB	ASP	A	846	73.294	36.787	2.390	1.00	100.00
ATOM	251	CG	ASP	A	846	74.415	37.685	1.842	1.00	100.00
ATOM	252	OD1	ASP	A	846	74.632	37.694	0.607	1.00	100.00
ATOM	253	OD2	ASP	A	846	75.083	38.376	2.650	1.00	100.00
ATOM	255	N	GLY	A	847	69.992	35.836	1.082	1.00	99.53
ATOM	256	CA	GLY	A	847	68.923	34.870	1.231	1.00	99.53
ATOM	257	C	GLY	A	847	68.008	35.367	2.347	1.00	99.53
ATOM	258	O	GLY	A	847	68.509	35.974	3.302	1.00	99.53
ATOM	260	N	LEU	A	848	66.694	35.120	2.228	1.00	93.78
ATOM	261	CA	LEU	A	848	65.670	35.542	3.212	1.00	93.78
ATOM	262	C	LEU	A	848	65.095	36.935	2.949	1.00	93.78
ATOM	263	O	LEU	A	848	65.825	37.878	2.662	1.00	93.78
ATOM	264	CB	LEU	A	848	66.215	35.504	4.654	1.00	100.00
ATOM	265	CG	LEU	A	848	66.931	36.752	5.223	1.00	100.00
ATOM	266	CD1	LEU	A	848	65.937	37.849	5.552	1.00	100.00
ATOM	267	CD2	LEU	A	848	67.719	36.377	6.472	1.00	100.00
ATOM	269	N	ARG	A	849	63.781	37.063	3.070	1.00	80.14
ATOM	270	CA	ARG	A	849	63.127	38.347	2.855	1.00	80.14
ATOM	271	C	ARG	A	849	62.191	38.669	4.013	1.00	80.14
ATOM	272	O	ARG	A	849	61.629	37.748	4.612	1.00	80.14

FIG. .6D

ATOM	273	CB	ARG	A	849	62.320	38.327	1.561	1.00 99.23
ATOM	274	CG	ARG	A	849	61.390	37.148	1.452	1.00 99.23
ATOM	275	CD	ARG	A	849	60.021	37.392	2.081	1.00 99.23
ATOM	276	NE	ARG	A	849	59.022	36.466	1.540	1.00 99.23
ATOM	277	CZ	ARG	A	849	58.743	35.268	2.050	1.00 99.23
ATOM	278	NH1	ARG	A	849	59.379	34.826	3.127	1.00 99.23
ATOM	279	NH2	ARG	A	849	57.830	34.504	1.475	1.00 99.23
ATOM	286	N	MET	A	850	62.041	39.958	4.350	1.00 26.65
ATOM	287	CA	MET	A	850	61.122	40.332	5.425	1.00 26.65
ATOM	288	C	MET	A	850	60.680	41.820	5.406	1.00 26.65
ATOM	289	O	MET	A	850	60.502	42.468	4.345	1.00 26.65
ATOM	290	CB	MET	A	850	61.743	39.999	6.780	1.00 99.56
ATOM	291	CG	MET	A	850	63.156	39.475	6.689	1.00 99.56
ATOM	292	SD	MET	A	850	64.190	40.566	5.745	1.00 99.56
ATOM	293	CE	MET	A	850	65.522	40.771	6.902	1.00 99.56
ATOM	295	N	ASP	A	851	60.515	42.341	6.612	1.00 27.82
ATOM	296	CA	ASP	A	851	60.156	43.721	6.812	1.00 27.82
ATOM	297	C	ASP	A	851	61.331	44.534	7.280	1.00 27.82
ATOM	298	O	ASP	A	851	62.056	44.144	8.255	1.00 27.82
ATOM	299	CB	ASP	A	851	59.124	43.799	7.903	1.00 16.75
ATOM	300	CG	ASP	A	851	58.382	42.570	7.998	1.00 16.75
ATOM	301	OD1	ASP	A	851	58.147	42.049	6.837	1.00 16.75
ATOM	302	OD2	ASP	A	851	58.079	42.189	9.190	1.00 16.75
ATOM	304	N	ALA	A	852	61.420	45.691	6.635	1.00 37.08
ATOM	305	CA	ALA	A	852	62.400	46.719	6.887	1.00 37.08
ATOM	306	C	ALA	A	852	61.643	48.050	6.795	1.00 37.08
ATOM	307	O	ALA	A	852	60.764	48.247	5.950	1.00 37.08
ATOM	308	CB	ALA	A	852	63.471	46.663	5.835	1.00100.00
ATOM	310	N	ALA	A	853	61.955	48.986	7.663	1.00 97.32
ATOM	311	CA	ALA	A	853	61.303	50.269	7.528	1.00 97.32
ATOM	312	C	ALA	A	853	62.427	51.046	6.852	1.00 97.32
ATOM	313	O	ALA	A	853	63.501	51.201	7.415	1.00 97.32
ATOM	314	CB	ALA	A	853	60.947	50.824	8.895	1.00 15.46
ATOM	316	N	ILE	A	854	62.187	51.469	5.617	1.00 84.85
ATOM	317	CA	ILE	A	854	63.178	52.179	4.810	1.00 84.85
ATOM	318	C	ILE	A	854	63.221	53.682	4.985	1.00 84.85
ATOM	319	O	ILE	A	854	62.197	54.334	5.006	1.00 84.85
ATOM	320	CB	ILE	A	854	62.961	51.895	3.315	1.00 99.86
ATOM	321	CG1	ILE	A	854	63.540	50.538	2.948	1.00 99.86
ATOM	322	CG2	ILE	A	854	63.622	52.963	2.474	1.00 99.86
ATOM	323	CD1	ILE	A	854	63.707	49.610	4.109	1.00 99.86
ATOM	325	N	LYS	A	855	64.426	54.228	5.095	1.00100.00
ATOM	326	CA	LYS	A	855	64.602	55.666	5.249	1.00100.00
ATOM	327	C	LYS	A	855	65.867	56.179	4.602	1.00100.00
ATOM	328	O	LYS	A	855	66.915	55.567	4.710	1.00100.00
ATOM	329	CB	LYS	A	855	64.640	56.058	6.721	1.00100.00
ATOM	330	CG	LYS	A	855	65.352	57.373	6.977	1.00100.00
ATOM	331	CD	LYS	A	855	64.912	57.985	8.283	1.00100.00
ATOM	332	CE	LYS	A	855	65.371	57.143	9.459	1.00100.00
ATOM	333	NZ	LYS	A	855	66.801	57.366	9.812	1.00100.00
ATOM	338	N	ARG	A	856	65.751	57.314	3.927	1.00100.00
ATOM	339	CA	ARG	A	856	66.881	57.980	3.282	1.00100.00
ATOM	340	C	ARG	A	856	66.403	59.192	2.543	1.00100.00
ATOM	341	O	ARG	A	856	65.575	59.088	1.631	1.00100.00
ATOM	342	CB	ARG	A	856	67.602	57.089	2.279	1.00100.00
ATOM	343	CG	ARG	A	856	68.637	57.868	1.462	1.00100.00
ATOM	344	CD	ARG	A	856	68.118	58.410	0.090	1.00100.00

FIG. 6E

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ATOM    345  NE  ARG A 856      68.946  59.472  -0.512  1.00100.00
ATOM    346  CZ  ARG A 856      68.938  59.819  -1.801  1.00100.00
ATOM    347  NH1 ARG A 856      68.145  59.210  -2.674  1.00100.00
ATOM    348  NH2 ARG A 856      69.744  60.783  -2.222  1.00100.00
ATOM    355  N   MET A 857      66.951  60.337   2.922  1.00 39.23
ATOM    356  CA  MET A 857      66.567  61.616   2.275  1.00 39.23
ATOM    357  C   MET A 857      67.634  62.754   2.130  1.00 39.23
ATOM    358  O   MET A 857      68.221  63.225   3.157  1.00 39.23
ATOM    359  CB  MET A 857      65.320  62.179   2.983  1.00100.00
ATOM    360  CG  MET A 857      64.305  62.877   2.092  1.00100.00
ATOM    361  SD  MET A 857      63.851  64.409   2.908  1.00100.00
ATOM    362  CE  MET A 857      61.992  64.355   2.935  1.00100.00
ATOM    363  OXT MET A 857      67.842  63.172   0.963  1.00100.00
ATOM    365  N   ASP A 864      73.761  67.110  -3.548  1.00 99.95
ATOM    366  CA  ASP A 864      74.976  66.819  -4.360  1.00 99.95
ATOM    367  C   ASP A 864      76.224  67.493  -3.781  1.00 99.95
ATOM    368  O   ASP A 864      77.068  68.001  -4.530  1.00 99.95
ATOM    369  CB  ASP A 864      74.765  67.261  -5.839  1.00  2.00
ATOM    373  N   ASP A 865      76.338  67.492  -2.453  1.00100.00
ATOM    374  CA  ASP A 865      77.486  68.080  -1.760  1.00100.00
ATOM    375  C   ASP A 865      77.219  68.112  -0.267  1.00100.00
ATOM    376  O   ASP A 865      77.444  69.131   0.391  1.00100.00
ATOM    377  CB  ASP A 865      77.720  69.454  -2.255  1.00 53.42
ATOM    379  N   HIS A 866      76.752  66.983   0.263  1.00100.00
ATOM    380  CA  HIS A 866      76.397  66.853   1.678  1.00100.00
ATOM    381  C   HIS A 866      76.696  65.441   2.178  1.00100.00
ATOM    382  O   HIS A 866      75.859  64.777   2.805  1.00100.00
ATOM    383  CB  HIS A 866      74.905  67.144   1.848  1.00100.00
ATOM    384  CG  HIS A 866      74.036  66.378   0.896  1.00100.00
ATOM    385  ND1 HIS A 866      73.693  66.857  -0.350  1.00100.00
ATOM    386  CD2 HIS A 866      73.459  65.158   1.003  1.00100.00
ATOM    387  CE1 HIS A 866      72.943  65.965  -0.970  1.00100.00
ATOM    388  NE2 HIS A 866      72.787  64.925  -0.170  1.00100.00
ATOM    392  N   ARG A 867      77.912  64.998   1.913  1.00100.00
ATOM    393  CA  ARG A 867      78.335  63.673   2.300  1.00100.00
ATOM    394  C   ARG A 867      78.856  63.654   3.738  1.00100.00
ATOM    395  O   ARG A 867      80.061  63.597   3.985  1.00100.00
ATOM    396  CB  ARG A 867      79.393  63.206   1.310  1.00 99.71
ATOM    397  CG  ARG A 867      79.185  63.783  -0.098  1.00 99.71
ATOM    398  CD  ARG A 867      79.695  65.213  -0.213  1.00 99.71
ATOM    399  NE  ARG A 867      81.116  65.305   0.115  1.00 99.71
ATOM    400  CZ  ARG A 867      81.604  65.381   1.351  1.00 99.71
ATOM    401  NH1 ARG A 867      80.785  65.378   2.396  1.00 99.71
ATOM    402  NH2 ARG A 867      82.919  65.450   1.540  1.00 99.71
ATOM    409  N   ASP A 868      77.920  63.713   4.683  1.00 88.85
ATOM    410  CA  ASP A 868      78.239  63.706   6.112  1.00 88.85
ATOM    411  C   ASP A 868      77.969  62.278   6.646  1.00 88.85
ATOM    412  O   ASP A 868      78.558  61.850   7.655  1.00 88.85
ATOM    413  CB  ASP A 868      77.368  64.758   6.870  1.00 67.57
ATOM    414  CG  ASP A 868      77.674  66.231   6.460  1.00 67.57
ATOM    415  OD1 ASP A 868      78.671  66.496   5.753  1.00 67.57
ATOM    416  OD2 ASP A 868      76.914  67.142   6.852  1.00 67.57
ATOM    418  N   PHE A 869      77.097  61.545   5.943  1.00100.00
ATOM    419  CA  PHE A 869      76.719  60.176   6.322  1.00100.00
ATOM    420  C   PHE A 869      77.809  59.128   6.086  1.00100.00
ATOM    421  O   PHE A 869      78.433  59.091   5.017  1.00100.00
ATOM    422  CB  PHE A 869      75.431  59.745   5.595  1.00 98.24
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FIG. 6F

ATOM	423	CG	PHE	A	869	75.346	60.207	4.164	1.00 98.24
ATOM	424	CD1	PHE	A	869	74.434	61.186	3.789	1.00 98.24
ATOM	425	CD2	PHE	A	869	76.165	59.652	3.186	1.00 98.24
ATOM	426	CE1	PHE	A	869	74.341	61.604	2.457	1.00 98.24
ATOM	427	CE2	PHE	A	869	76.078	60.063	1.854	1.00 98.24
ATOM	428	CZ	PHE	A	869	75.166	61.038	1.492	1.00 98.24
ATOM	430	N	ALA	A	870	78.007	58.287	7.106	1.00100.00
ATOM	431	CA	ALA	A	870	79.005	57.205	7.146	1.00100.00
ATOM	432	C	ALA	A	870	79.570	57.201	8.564	1.00100.00
ATOM	433	O	ALA	A	870	80.736	56.892	8.807	1.00100.00
ATOM	434	CB	ALA	A	870	80.131	57.437	6.134	1.00100.00
ATOM	436	N	GLY	A	871	78.706	57.575	9.490	1.00100.00
ATOM	437	CA	GLY	A	871	79.058	57.626	10.888	1.00100.00
ATOM	438	C	GLY	A	871	77.783	57.234	11.591	1.00100.00
ATOM	439	O	GLY	A	871	77.802	56.636	12.662	1.00100.00
ATOM	441	N	GLU	A	872	76.656	57.592	10.987	1.00100.00
ATOM	442	CA	GLU	A	872	75.384	57.210	11.564	1.00100.00
ATOM	443	C	GLU	A	872	75.581	55.695	11.584	1.00100.00
ATOM	444	O	GLU	A	872	75.628	55.083	12.655	1.00100.00
ATOM	445	CB	GLU	A	872	74.200	57.613	10.651	1.00 99.93
ATOM	446	CG	GLU	A	872	73.244	58.668	11.260	1.00 99.93
ATOM	447	CD	GLU	A	872	71.754	58.458	10.919	1.00 99.93
ATOM	448	OE1	GLU	A	872	71.434	57.633	10.040	1.00 99.93
ATOM	449	OE2	GLU	A	872	70.894	59.128	11.532	1.00 99.93
ATOM	451	N	LEU	A	873	75.773	55.121	10.389	1.00 77.06
ATOM	452	CA	LEU	A	873	75.982	53.683	10.215	1.00 77.06
ATOM	453	C	LEU	A	873	77.167	53.198	11.046	1.00 77.06
ATOM	454	O	LEU	A	873	77.384	51.998	11.180	1.00 77.06
ATOM	455	CB	LEU	A	873	76.202	53.366	8.746	1.00 96.97
ATOM	457	N	GLU	A	874	77.920	54.142	11.612	1.00 98.87
ATOM	458	CA	GLU	A	874	79.091	53.832	12.423	1.00 98.87
ATOM	459	C	GLU	A	874	78.740	53.585	13.890	1.00 98.87
ATOM	460	O	GLU	A	874	79.072	52.546	14.449	1.00 98.87
ATOM	461	CB	GLU	A	874	80.107	54.954	12.306	1.00 56.03
ATOM	463	N	VAL	A	875	78.096	54.541	14.543	1.00100.00
ATOM	464	CA	VAL	A	875	77.725	54.320	15.936	1.00100.00
ATOM	465	C	VAL	A	875	76.577	53.312	15.875	1.00100.00
ATOM	466	O	VAL	A	875	76.533	52.370	16.654	1.00100.00
ATOM	467	CB	VAL	A	875	77.279	55.629	16.582	1.00100.00
ATOM	469	N	LEU	A	876	75.678	53.520	14.911	1.00 63.64
ATOM	470	CA	LEU	A	876	74.515	52.662	14.649	1.00 63.64
ATOM	471	C	LEU	A	876	74.825	51.155	14.638	1.00 63.64
ATOM	472	O	LEU	A	876	73.935	50.359	14.292	1.00 63.64
ATOM	473	CB	LEU	A	876	73.914	53.005	13.267	1.00 36.83
ATOM	474	CG	LEU	A	876	72.851	54.076	12.997	1.00 36.83
ATOM	475	CD1	LEU	A	876	72.028	53.665	11.807	1.00 36.83
ATOM	476	CD2	LEU	A	876	71.987	54.260	14.181	1.00 36.83
ATOM	478	N	CYS	A	877	76.072	50.786	14.978	1.00 75.85
ATOM	479	CA	CYS	A	877	76.570	49.391	14.973	1.00 75.85
ATOM	480	C	CYS	A	877	76.791	48.697	16.317	1.00 75.85
ATOM	481	O	CYS	A	877	75.965	47.904	16.771	1.00 75.85
ATOM	482	CB	CYS	A	877	77.890	49.343	14.202	1.00 82.25
ATOM	483	SG	CYS	A	877	78.205	50.859	13.250	1.00 82.25
ATOM	485	N	LYS	A	878	77.947	48.968	16.913	1.00100.00
ATOM	486	CA	LYS	A	878	78.334	48.400	18.202	1.00100.00
ATOM	487	C	LYS	A	878	77.159	48.295	19.186	1.00100.00
ATOM	488	O	LYS	A	878	77.237	47.565	20.178	1.00100.00

ATOM	489	CB	LYS	A	878	79.460	49.251	18.826	1.00 99.60
ATOM	490	CG	LYS	A	878	80.588	49.643	17.842	1.00 99.60
ATOM	491	CD	LYS	A	878	80.814	51.160	17.739	1.00 99.60
ATOM	492	CE	LYS	A	878	81.022	51.598	16.292	1.00 99.60
ATOM	493	NZ	LYS	A	878	82.152	52.567	16.077	1.00 99.60
ATOM	498	N	LEU	A	879	76.079	49.024	18.905	1.00 99.14
ATOM	499	CA	LEU	A	879	74.905	49.034	19.762	1.00 99.14
ATOM	500	C	LEU	A	879	73.664	48.687	18.953	1.00 99.14
ATOM	501	O	LEU	A	879	72.574	48.526	19.488	1.00 99.14
ATOM	502	CB	LEU	A	879	74.748	50.416	20.401	1.00 99.96
ATOM	503	CG	LEU	A	879	74.125	51.546	19.579	1.00 99.96
ATOM	504	CD1	LEU	A	879	74.530	52.863	20.154	1.00 99.96
ATOM	505	CD2	LEU	A	879	74.555	51.454	18.135	1.00 99.96
ATOM	507	N	GLY	A	880	73.840	48.593	17.647	1.00 74.75
ATOM	508	CA	GLY	A	880	72.737	48.256	16.775	1.00 74.75
ATOM	509	C	GLY	A	880	71.778	47.281	17.406	1.00 74.75
ATOM	510	O	GLY	A	880	70.589	47.458	17.285	1.00 74.75
ATOM	512	N	HIS	A	881	72.288	46.243	18.067	1.00100.00
ATOM	513	CA	HIS	A	881	71.428	45.246	18.700	1.00100.00
ATOM	514	C	HIS	A	881	71.274	45.583	20.172	1.00100.00
ATOM	515	O	HIS	A	881	71.798	46.571	20.661	1.00100.00
ATOM	516	CB	HIS	A	881	71.989	43.818	18.514	1.00 80.74
ATOM	517	CG	HIS	A	881	71.360	42.778	19.401	1.00 80.74
ATOM	518	ND1	HIS	A	881	70.116	42.234	19.155	1.00 80.74
ATOM	519	CD2	HIS	A	881	71.778	42.230	20.573	1.00 80.74
ATOM	520	CE1	HIS	A	881	69.792	41.404	20.133	1.00 80.74
ATOM	521	NE2	HIS	A	881	70.783	41.384	21.007	1.00 80.74
ATOM	525	N	HIS	A	882	70.539	44.718	20.846	1.00 5.03
ATOM	526	CA	HIS	A	882	70.126	44.779	22.266	1.00 5.03
ATOM	527	C	HIS	A	882	68.572	44.646	22.018	1.00 5.03
ATOM	528	O	HIS	A	882	67.998	45.211	20.996	1.00 5.03
ATOM	529	CB	HIS	A	882	70.487	46.161	22.887	1.00 36.20
ATOM	530	CG	HIS	A	882	70.085	46.316	24.322	1.00 36.20
ATOM	531	ND1	HIS	A	882	68.786	46.169	24.753	1.00 36.20
ATOM	532	CD2	HIS	A	882	70.816	46.553	25.432	1.00 36.20
ATOM	533	CE1	HIS	A	882	68.731	46.302	26.066	1.00 36.20
ATOM	534	NE2	HIS	A	882	69.949	46.535	26.504	1.00 36.20
ATOM	538	N	PRO	A	883	67.875	43.928	22.885	1.00 18.79
ATOM	539	CA	PRO	A	883	66.444	43.868	22.564	1.00 18.79
ATOM	540	C	PRO	A	883	65.806	45.252	22.201	1.00 18.79
ATOM	541	O	PRO	A	883	65.014	45.404	21.188	1.00 18.79
ATOM	542	CB	PRO	A	883	65.804	43.294	23.829	1.00 41.14
ATOM	543	CG	PRO	A	883	66.946	43.069	24.810	1.00 41.14
ATOM	544	CD	PRO	A	883	68.231	43.209	24.107	1.00 41.14
ATOM	545	N	ASN	A	884	66.245	46.252	22.975	1.00 21.27
ATOM	546	CA	ASN	A	884	65.656	47.545	22.910	1.00 21.27
ATOM	547	C	ASN	A	884	66.055	48.782	22.174	1.00 21.27
ATOM	548	O	ASN	A	884	65.930	49.811	22.738	1.00 21.27
ATOM	549	CB	ASN	A	884	65.371	47.916	24.332	1.00 47.99
ATOM	550	CG	ASN	A	884	64.926	46.747	25.093	1.00 47.99
ATOM	551	OD1	ASN	A	884	65.360	46.508	26.173	1.00 47.99
ATOM	552	ND2	ASN	A	884	64.056	45.990	24.504	1.00 47.99
ATOM	556	N	ILE	A	885	66.421	48.685	20.906	1.00 2.00
ATOM	557	CA	ILE	A	885	66.784	49.799	20.139	1.00 2.00
ATOM	558	C	ILE	A	885	66.578	49.337	18.712	1.00 2.00
ATOM	559	O	ILE	A	885	67.324	48.601	18.278	1.00 2.00
ATOM	560	CB	ILE	A	885	68.282	50.142	20.404	1.00 5.30

FIG. 6H

ATOM	562	CG1	ILE	A	885	68.387	50.790	21.774	1.00	5.30
ATOM	562	CG2	ILE	A	885	68.946	51.096	19.301	1.00	5.30
ATOM	563	CD1	ILE	A	885	69.834	51.062	22.137	1.00	5.30
ATOM	565	N	ILE	A	886	65.634	49.811	17.931	1.00	41.79
ATOM	566	CA	ILE	A	886	65.528	49.296	16.564	1.00	41.79
ATOM	567	C	ILE	A	886	66.883	48.887	15.937	1.00	41.79
ATOM	568	O	ILE	A	886	67.899	49.217	16.450	1.00	41.79
ATOM	569	CB	ILE	A	886	64.769	50.316	15.671	1.00	97.62
ATOM	570	CG1	ILE	A	886	63.737	49.563	14.817	1.00	97.62
ATOM	571	CG2	ILE	A	886	65.742	51.141	14.871	1.00	97.62
ATOM	572	CD1	ILE	A	886	62.833	50.438	14.004	1.00	97.62
ATOM	574	N	ASN	A	887	66.915	48.190	14.817	1.00	58.02
ATOM	575	CA	ASN	A	887	68.191	47.751	14.300	1.00	58.02
ATOM	576	C	ASN	A	887	68.481	48.230	12.940	1.00	58.02
ATOM	577	O	ASN	A	887	67.635	48.811	12.321	1.00	58.02
ATOM	578	CB	ASN	A	887	68.237	46.228	14.269	1.00	61.11
ATOM	579	CG	ASN	A	887	69.626	45.688	14.460	1.00	61.11
ATOM	580	OD1	ASN	A	887	70.307	45.367	13.505	1.00	61.11
ATOM	581	ND2	ASN	A	887	70.050	45.584	15.711	1.00	61.11
ATOM	585	N	LEU	A	888	69.688	47.945	12.467	1.00	100.00
ATOM	586	CA	LEU	A	888	70.097	48.313	11.122	1.00	100.00
ATOM	587	C	LEU	A	888	70.158	47.037	10.282	1.00	100.00
ATOM	588	O	LEU	A	888	71.039	46.202	10.444	1.00	100.00
ATOM	589	CB	LEU	A	888	71.467	48.993	11.131	1.00	100.00
ATOM	590	CG	LEU	A	888	72.068	49.217	9.743	1.00	100.00
ATOM	591	CD1	LEU	A	888	72.054	50.676	9.410	1.00	100.00
ATOM	592	CD2	LEU	A	888	73.475	48.686	9.699	1.00	100.00
ATOM	594	N	LEU	A	889	69.191	46.880	9.398	1.00	73.18
ATOM	595	CA	LEU	A	889	69.128	45.721	8.530	1.00	73.18
ATOM	596	C	LEU	A	889	70.044	45.860	7.290	1.00	73.18
ATOM	597	O	LEU	A	889	70.737	44.920	6.926	1.00	73.18
ATOM	598	CB	LEU	A	889	67.666	45.500	8.102	1.00	10.03
ATOM	599	CG	LEU	A	889	66.628	44.729	9.010	1.00	10.03
ATOM	600	CD1	LEU	A	889	66.180	43.517	8.146	1.00	10.03
ATOM	601	CD2	LEU	A	889	67.147	44.336	10.432	1.00	10.03
ATOM	603	N	GLY	A	890	70.058	47.028	6.651	1.00	100.00
ATOM	604	CA	GLY	A	890	70.898	47.201	5.475	1.00	100.00
ATOM	605	C	GLY	A	890	71.057	48.582	4.845	1.00	100.00
ATOM	606	O	GLY	A	890	70.515	49.581	5.319	1.00	100.00
ATOM	608	N	ALA	A	891	71.829	48.616	3.758	1.00	93.61
ATOM	609	CA	ALA	A	891	72.124	49.833	2.992	1.00	93.61
ATOM	610	C	ALA	A	891	73.125	49.438	1.929	1.00	93.61
ATOM	611	O	ALA	A	891	73.999	48.626	2.223	1.00	93.61
ATOM	612	CB	ALA	A	891	72.763	50.871	3.886	1.00	28.61
ATOM	614	N	CYS	A	892	73.033	49.985	0.715	1.00	100.00
ATOM	615	CA	CYS	A	892	74.034	49.635	-0.306	1.00	100.00
ATOM	616	C	CYS	A	892	74.789	50.793	-0.956	1.00	100.00
ATOM	617	O	CYS	A	892	75.934	51.073	-0.606	1.00	100.00
ATOM	618	CB	CYS	A	892	73.432	48.787	-1.429	1.00	100.00
ATOM	619	SG	CYS	A	892	74.641	48.356	-2.757	1.00	100.00
ATOM	621	N	GLU	A	893	74.134	51.447	-1.914	1.00	85.23
ATOM	622	CA	GLU	A	893	74.715	52.555	-2.679	1.00	85.23
ATOM	623	C	GLU	A	893	73.816	52.794	-3.880	1.00	85.23
ATOM	624	O	GLU	A	893	74.228	52.512	-5.011	1.00	85.23
ATOM	625	CB	GLU	A	893	76.108	52.176	-3.222	1.00	100.00
ATOM	626	CG	GLU	A	893	77.267	53.065	-2.785	1.00	100.00
ATOM	627	CD	GLU	A	893	78.487	52.246	-2.386	1.00	100.00

FIG. 6I

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ATOM    628  OE1 GLU A 893      79.029  51.535  -3.266  1.00100.00
ATOM    629  OE2 GLU A 893      78.893  52.307  -1.197  1.00100.00
ATOM    631  N   HIS A 894      72.602  53.293  -3.664  1.00100.00
ATOM    632  CA  HIS A 894      71.731  53.508  -4.810  1.00100.00
ATOM    633  C   HIS A 894      71.885  54.855  -5.463  1.00100.00
ATOM    634  O   HIS A 894      71.106  55.770  -5.181  1.00100.00
ATOM    635  CB  HIS A 894      70.261  53.338  -4.477  1.00100.00
ATOM    636  CG  HIS A 894      69.370  53.597  -5.652  1.00100.00
ATOM    637  ND1 HIS A 894      68.309  54.476  -5.610  1.00100.00
ATOM    638  CD2 HIS A 894      69.419  53.128  -6.922  1.00100.00
ATOM    639  CE1 HIS A 894      67.743  54.539  -6.802  1.00100.00
ATOM    640  NE2 HIS A 894      68.397  53.729  -7.615  1.00100.00
ATOM    644  N   ARG A 895      72.888  54.950  -6.340  1.00100.00
ATOM    645  CA  ARG A 895      73.176  56.161  -7.090  1.00100.00
ATOM    646  C   ARG A 895      72.331  57.309  -6.481  1.00100.00
ATOM    647  O   ARG A 895      71.194  57.562  -6.910  1.00100.00
ATOM    648  CB  ARG A 895      72.842  55.883  -8.571  1.00 36.65
ATOM    649  CG  ARG A 895      73.711  54.767  -9.229  1.00 36.65
ATOM    650  CD  ARG A 895      73.012  54.079 -10.421  1.00 36.65
ATOM    651  NE  ARG A 895      73.587  54.370 -11.738  1.00 36.65
ATOM    652  CZ  ARG A 895      74.382  53.546 -12.451  1.00 36.65
ATOM    653  NH1 ARG A 895      74.735  52.315 -11.986  1.00 36.65
ATOM    654  NH2 ARG A 895      74.848  53.963 -13.644  1.00 36.65
ATOM    661  N   GLY A 896      72.901  57.979  -5.469  1.00 33.20
ATOM    662  CA  GLY A 896      72.190  59.016  -4.751  1.00 33.20
ATOM    663  C   GLY A 896      71.918  58.455  -3.348  1.00 33.20
ATOM    664  O   GLY A 896      70.779  58.462  -2.847  1.00 33.20
ATOM    666  N   TYR A 897      72.971  57.947  -2.705  1.00 98.45
ATOM    667  CA  TYR A 897      72.864  57.372  -1.356  1.00 98.45
ATOM    668  C   TYR A 897      72.959  55.835  -1.387  1.00 98.45
ATOM    669  O   TYR A 897      73.599  55.240  -2.258  1.00 98.45
ATOM    670  CB  TYR A 897      71.532  57.786  -0.716  1.00100.00
ATOM    671  CG  TYR A 897      71.522  58.208   0.734  1.00100.00
ATOM    672  CD1 TYR A 897      71.152  59.511   1.080  1.00100.00
ATOM    673  CD2 TYR A 897      71.631  57.268   1.756  1.00100.00
ATOM    674  CE1 TYR A 897      70.860  59.866   2.391  1.00100.00
ATOM    675  CE2 TYR A 897      71.345  57.604   3.074  1.00100.00
ATOM    676  CZ  TYR A 897      70.947  58.908   3.389  1.00100.00
ATOM    677  OH  TYR A 897      70.582  59.246   4.682  1.00100.00
ATOM    680  N   LEU A 898      72.293  55.212  -0.419  1.00100.00
ATOM    681  CA  LEU A 898      72.272  53.765  -0.258  1.00100.00
ATOM    682  C   LEU A 898      70.983  53.363   0.469  1.00100.00
ATOM    683  O   LEU A 898      70.810  52.197   0.836  1.00100.00
ATOM    684  CB  LEU A 898      73.495  53.328   0.551  1.00 67.92
ATOM    686  N   TYR A 899      70.097  54.345   0.668  1.00100.00
ATOM    687  CA  TYR A 899      68.813  54.169   1.347  1.00100.00
ATOM    688  C   TYR A 899      68.976  53.434   2.680  1.00100.00
ATOM    689  O   TYR A 899      70.090  53.252   3.153  1.00100.00
ATOM    690  CB  TYR A 899      67.840  53.420   0.434  1.00 99.94
ATOM    691  CG  TYR A 899      67.265  54.259  -0.694  1.00 99.94
ATOM    692  CD1 TYR A 899      67.218  53.770  -2.004  1.00 99.94
ATOM    693  CD2 TYR A 899      66.738  55.531  -0.454  1.00 99.94
ATOM    694  CE1 TYR A 899      66.662  54.519  -3.044  1.00 99.94
ATOM    695  CE2 TYR A 899      66.176  56.295  -1.493  1.00 99.94
ATOM    696  CZ  TYR A 899      66.143  55.778  -2.780  1.00 99.94
ATOM    697  OH  TYR A 899      65.580  56.509  -3.792  1.00 99.94
ATOM    700  N   LEU A 900      67.876  53.017   3.300  1.00 99.32
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FIG. 6J

ATOM	701	CA	LEU	A	900	67.987	52.305	4.573	1.00 99.32
ATOM	702	C	LEU	A	900	67.119	51.071	4.770	1.00 99.32
ATOM	703	O	LEU	A	900	66.306	50.702	3.933	1.00 99.32
ATOM	704	CB	LEU	A	900	67.755	53.258	5.752	1.00 72.65
ATOM	705	CG	LEU	A	900	68.911	53.350	6.752	1.00 72.65
ATOM	706	CD1	LEU	A	900	70.175	52.843	6.059	1.00 72.65
ATOM	707	CD2	LEU	A	900	69.096	54.792	7.259	1.00 72.65
ATOM	709	N	ALA	A	901	67.330	50.439	5.912	1.00100.00
ATOM	710	CA	ALA	A	901	66.617	49.244	6.288	1.00100.00
ATOM	711	C	ALA	A	901	66.802	49.053	7.774	1.00100.00
ATOM	712	O	ALA	A	901	67.774	48.484	8.231	1.00100.00
ATOM	713	CB	ALA	A	901	67.152	48.049	5.537	1.00100.00
ATOM	715	N	ILE	A	902	65.840	49.575	8.510	1.00 33.23
ATOM	716	CA	ILE	A	902	65.773	49.510	9.964	1.00 33.23
ATOM	717	C	ILE	A	902	64.912	48.295	10.352	1.00 33.23
ATOM	718	O	ILE	A	902	63.988	47.959	9.648	1.00 33.23
ATOM	719	CB	ILE	A	902	65.130	50.817	10.474	1.00 58.03
ATOM	720	CG1	ILE	A	902	65.930	51.992	9.960	1.00 58.03
ATOM	721	CG2	ILE	A	902	65.107	50.870	11.955	1.00 58.03
ATOM	722	CD1	ILE	A	902	67.193	52.207	10.738	1.00 58.03
ATOM	724	N	GLU	A	903	65.256	47.622	11.440	1.00 37.33
ATOM	725	CA	GLU	A	903	64.468	46.507	11.912	1.00 37.33
ATOM	726	C	GLU	A	903	63.079	47.051	11.790	1.00 37.33
ATOM	727	O	GLU	A	903	62.856	48.198	12.081	1.00 37.33
ATOM	728	CB	GLU	A	903	64.732	46.216	13.388	1.00 74.67
ATOM	729	CG	GLU	A	903	63.667	45.362	14.022	1.00 74.67
ATOM	730	CD	GLU	A	903	63.757	45.302	15.525	1.00 74.67
ATOM	731	OE1	GLU	A	903	62.771	44.921	16.178	1.00 74.67
ATOM	732	OE2	GLU	A	903	64.809	45.637	16.072	1.00 74.67
ATOM	734	N	TYR	A	904	62.137	46.221	11.362	1.00 98.95
ATOM	735	CA	TYR	A	904	60.765	46.667	11.209	1.00 98.95
ATOM	736	C	TYR	A	904	59.912	46.319	12.435	1.00 98.95
ATOM	737	O	TYR	A	904	59.998	45.210	12.968	1.00 98.95
ATOM	738	CB	TYR	A	904	60.187	46.064	9.939	1.00 65.21
ATOM	739	CG	TYR	A	904	58.741	46.366	9.749	1.00 65.21
ATOM	740	CD1	TYR	A	904	58.343	47.461	9.002	1.00 65.21
ATOM	741	CD2	TYR	A	904	57.760	45.602	10.367	1.00 65.21
ATOM	742	CE1	TYR	A	904	56.994	47.797	8.878	1.00 65.21
ATOM	743	CE2	TYR	A	904	56.418	45.929	10.249	1.00 65.21
ATOM	744	CZ	TYR	A	904	56.046	47.029	9.500	1.00 65.21
ATOM	745	OH	TYR	A	904	54.736	47.335	9.321	1.00 65.21
ATOM	748	N	ALA	A	905	59.103	47.287	12.877	1.00 44.07
ATOM	749	CA	ALA	A	905	58.241	47.148	14.049	1.00 44.07
ATOM	750	C	ALA	A	905	56.742	46.973	13.670	1.00 44.07
ATOM	751	O	ALA	A	905	56.091	47.865	13.125	1.00 44.07
ATOM	752	CB	ALA	A	905	58.459	48.326	14.943	1.00 44.16
ATOM	754	N	PRO	A	906	56.169	45.798	13.983	1.00 95.76
ATOM	755	CA	PRO	A	906	54.773	45.513	13.643	1.00 95.76
ATOM	756	C	PRO	A	906	53.627	46.336	14.226	1.00 95.76
ATOM	757	O	PRO	A	906	52.547	46.358	13.656	1.00 95.76
ATOM	758	CB	PRO	A	906	54.642	44.022	13.956	1.00 74.50
ATOM	759	CG	PRO	A	906	55.605	43.816	15.072	1.00 74.50
ATOM	760	CD	PRO	A	906	56.773	44.682	14.734	1.00 74.50
ATOM	761	N	HIS	A	907	53.838	47.018	15.336	1.00 75.88
ATOM	762	CA	HIS	A	907	52.751	47.792	15.909	1.00 75.88
ATOM	763	C	HIS	A	907	52.942	49.300	15.917	1.00 75.88
ATOM	764	O	HIS	A	907	52.370	49.979	16.754	1.00 75.88

FIG. 6K

ATOM	765	CB	HIS	A	907	52.491	47.321	17.327	1.00	58.13
ATOM	766	CG	HIS	A	907	52.494	45.839	17.465	1.00	58.13
ATOM	767	ND1	HIS	A	907	52.400	44.991	16.387	1.00	58.13
ATOM	768	CD2	HIS	A	907	52.595	45.049	18.552	1.00	58.13
ATOM	769	CE1	HIS	A	907	52.442	43.741	16.805	1.00	58.13
ATOM	770	NE2	HIS	A	907	52.563	43.750	18.117	1.00	58.13
ATOM	774	N	GLY	A	908	53.744	49.827	15.004	1.00	99.49
ATOM	775	CA	GLY	A	908	53.952	51.258	14.965	1.00	99.49
ATOM	776	C	GLY	A	908	54.688	51.796	16.168	1.00	99.49
ATOM	777	O	GLY	A	908	55.536	51.126	16.736	1.00	99.49
ATOM	779	N	ASN	A	909	54.345	53.015	16.565	1.00	37.36
ATOM	780	CA	ASN	A	909	54.995	53.672	17.686	1.00	37.36
ATOM	781	C	ASN	A	909	54.274	53.675	18.970	1.00	37.36
ATOM	782	O	ASN	A	909	53.091	53.524	19.093	1.00	37.36
ATOM	783	CB	ASN	A	909	55.422	55.139	17.378	1.00	21.80
ATOM	784	CG	ASN	A	909	54.300	56.174	17.594	1.00	21.80
ATOM	785	OD1	ASN	A	909	54.091	57.036	16.763	1.00	21.80
ATOM	786	ND2	ASN	A	909	53.611	56.094	18.714	1.00	21.80
ATOM	790	N	LEU	A	910	55.043	53.958	19.971	1.00	6.05
ATOM	791	CA	LEU	A	910	54.505	53.895	21.258	1.00	6.05
ATOM	792	C	LEU	A	910	53.372	54.836	21.506	1.00	6.05
ATOM	793	O	LEU	A	910	52.558	54.488	22.290	1.00	6.05
ATOM	794	CB	LEU	A	910	55.629	53.964	22.304	1.00	22.43
ATOM	795	CG	LEU	A	910	55.112	53.756	23.738	1.00	22.43
ATOM	796	CD1	LEU	A	910	54.795	52.285	23.989	1.00	22.43
ATOM	797	CD2	LEU	A	910	56.128	54.383	24.829	1.00	22.43
ATOM	799	N	LEU	A	911	53.269	56.034	20.959	1.00	53.76
ATOM	800	CA	LEU	A	911	52.062	56.772	21.333	1.00	53.76
ATOM	801	C	LEU	A	911	50.801	56.136	20.690	1.00	53.76
ATOM	802	O	LEU	A	911	49.969	55.583	21.406	1.00	53.76
ATOM	803	CB	LEU	A	911	52.158	58.265	20.991	1.00	2.16
ATOM	804	CG	LEU	A	911	51.350	59.370	21.692	1.00	2.16
ATOM	805	CD1	LEU	A	911	51.622	59.513	23.075	1.00	2.16
ATOM	806	CD2	LEU	A	911	51.612	60.569	20.997	1.00	2.16
ATOM	808	N	ASP	A	912	50.666	56.165	19.363	1.00	37.67
ATOM	809	CA	ASP	A	912	49.481	55.594	18.764	1.00	37.67
ATOM	810	C	ASP	A	912	49.087	54.287	19.391	1.00	37.67
ATOM	811	O	ASP	A	912	48.010	54.116	19.875	1.00	37.67
ATOM	812	CB	ASP	A	912	49.652	55.383	17.285	1.00	2.00
ATOM	813	CG	ASP	A	912	49.965	56.675	16.516	1.00	2.00
ATOM	814	OD1	ASP	A	912	49.929	56.718	15.258	1.00	2.00
ATOM	815	OD2	ASP	A	912	50.263	57.647	17.195	1.00	2.00
ATOM	817	N	PHE	A	913	49.977	53.341	19.403	1.00	21.37
ATOM	818	CA	PHE	A	913	49.659	52.056	19.975	1.00	21.37
ATOM	819	C	PHE	A	913	49.216	52.291	21.331	1.00	21.37
ATOM	820	O	PHE	A	913	48.338	51.566	21.787	1.00	21.37
ATOM	821	CB	PHE	A	913	50.826	51.097	19.956	1.00	2.23
ATOM	822	CG	PHE	A	913	50.639	49.861	20.776	1.00	2.23
ATOM	823	CD1	PHE	A	913	50.389	48.681	20.185	1.00	2.23
ATOM	824	CD2	PHE	A	913	50.826	49.886	22.142	1.00	2.23
ATOM	825	CE1	PHE	A	913	50.330	47.610	20.870	1.00	2.23
ATOM	826	CE2	PHE	A	913	50.749	48.684	22.902	1.00	2.23
ATOM	827	CZ	PHE	A	913	50.503	47.593	22.238	1.00	2.23
ATOM	829	N	LEU	A	914	49.753	53.295	22.003	1.00	34.44
ATOM	830	CA	LEU	A	914	49.233	53.552	23.340	1.00	34.44
ATOM	831	C	LEU	A	914	47.770	54.028	23.202	1.00	34.44
ATOM	832	O	LEU	A	914	46.927	53.718	24.017	1.00	34.44

FIG. 6L

ATOM	833	CB	LEU	A	914	50.089	54.600	24.053	1.00	99.33
ATOM	834	CG	LEU	A	914	51.192	54.077	24.972	1.00	99.33
ATOM	835	CD1	LEU	A	914	52.365	55.032	24.979	1.00	99.33
ATOM	836	CD2	LEU	A	914	50.633	53.912	26.367	1.00	99.33
ATOM	838	N	ARG	A	915	47.489	54.720	22.111	1.00	38.92
ATOM	839	CA	ARG	A	915	46.202	55.332	21.795	1.00	38.92
ATOM	840	C	ARG	A	915	45.058	54.463	21.348	1.00	38.92
ATOM	841	O	ARG	A	915	43.891	54.728	21.700	1.00	38.92
ATOM	842	CB	ARG	A	915	46.422	56.347	20.720	1.00	6.43
ATOM	843	CG	ARG	A	915	46.646	57.788	21.276	1.00	6.43
ATOM	844	CD	ARG	A	915	47.992	58.402	21.097	1.00	6.43
ATOM	845	NE	ARG	A	915	48.094	59.491	22.107	1.00	6.43
ATOM	846	CZ	ARG	A	915	48.254	60.805	21.838	1.00	6.43
ATOM	847	NH1	ARG	A	915	48.331	61.314	20.610	1.00	6.43
ATOM	848	NH2	ARG	A	915	48.468	61.590	22.822	1.00	6.43
ATOM	855	N	LYS	A	916	45.399	53.475	20.520	1.00	22.32
ATOM	856	CA	LYS	A	916	44.513	52.462	20.007	1.00	22.32
ATOM	857	C	LYS	A	916	44.158	51.432	21.156	1.00	22.32
ATOM	858	O	LYS	A	916	43.680	50.278	20.864	1.00	22.32
ATOM	859	CB	LYS	A	916	45.275	51.740	18.908	1.00	23.97
ATOM	860	CG	LYS	A	916	46.735	51.281	19.327	1.00	23.97
ATOM	861	CD	LYS	A	916	46.899	50.099	20.472	1.00	23.97
ATOM	862	CE	LYS	A	916	46.886	48.726	19.880	1.00	23.97
ATOM	863	NZ	LYS	A	916	46.600	48.934	18.374	1.00	23.97
ATOM	868	N	SER	A	917	44.387	51.831	22.418	1.00	22.74
ATOM	869	CA	SER	A	917	44.179	51.001	23.600	1.00	22.74
ATOM	870	C	SER	A	917	43.034	51.499	24.516	1.00	22.74
ATOM	871	O	SER	A	917	42.627	50.829	25.545	1.00	22.74
ATOM	872	CB	SER	A	917	45.489	50.997	24.415	1.00	34.41
ATOM	873	OG	SER	A	917	45.310	50.676	25.795	1.00	34.41
ATOM	876	N	ARG	A	918	42.610	52.718	24.199	1.00	59.16
ATOM	877	CA	ARG	A	918	41.546	53.402	24.928	1.00	59.16
ATOM	878	C	ARG	A	918	40.240	52.937	24.293	1.00	59.16
ATOM	879	O	ARG	A	918	39.667	53.636	23.457	1.00	59.16
ATOM	880	CB	ARG	A	918	41.724	54.919	24.780	1.00	47.25
ATOM	881	CG	ARG	A	918	43.152	55.447	25.013	1.00	47.25
ATOM	882	CD	ARG	A	918	43.251	56.981	25.073	1.00	47.25
ATOM	883	NE	ARG	A	918	44.063	57.501	26.186	1.00	47.25
ATOM	884	CZ	ARG	A	918	44.349	58.794	26.368	1.00	47.25
ATOM	885	NH1	ARG	A	918	43.894	59.671	25.521	1.00	47.25
ATOM	886	NH2	ARG	A	918	45.092	59.226	27.374	1.00	47.25
ATOM	893	N	VAL	A	919	39.829	51.722	24.665	1.00	99.87
ATOM	894	CA	VAL	A	919	38.625	51.077	24.148	1.00	99.87
ATOM	895	C	VAL	A	919	37.442	52.049	24.208	1.00	99.87
ATOM	896	O	VAL	A	919	36.849	52.376	23.191	1.00	99.87
ATOM	897	CB	VAL	A	919	38.375	49.713	24.883	1.00	30.60
ATOM	898	CG1	VAL	A	919	39.007	48.626	24.110	1.00	30.60
ATOM	899	CG2	VAL	A	919	38.949	49.723	26.257	1.00	30.60
ATOM	901	N	LEU	A	920	37.111	52.497	25.405	1.00	36.31
ATOM	902	CA	LEU	A	920	36.115	53.513	25.648	1.00	36.31
ATOM	903	C	LEU	A	920	36.539	54.698	24.811	1.00	36.31
ATOM	904	O	LEU	A	920	37.065	55.646	25.312	1.00	36.31
ATOM	905	CB	LEU	A	920	36.201	53.928	27.088	1.00	11.95
ATOM	906	CG	LEU	A	920	34.951	54.248	27.902	1.00	11.95
ATOM	907	CD1	LEU	A	920	34.645	52.948	28.585	1.00	11.95
ATOM	908	CD2	LEU	A	920	35.117	55.350	28.954	1.00	11.95
ATOM	910	N	GLU	A	921	36.349	54.626	23.518	1.00	9.77

FIG. 6M

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ATOM    911  CA  GLU A 921      36.726  55.656  22.606  1.00  9.77
ATOM    912  C   GLU A 921      36.937  54.877  21.314  1.00  9.77
ATOM    913  O   GLU A 921      36.305  55.139  20.294  1.00  9.77
ATOM    914  CB  GLU A 921      38.009  56.321  23.076  1.00 41.44
ATOM    915  CG  GLU A 921      38.187  57.798  22.646  1.00 41.44
ATOM    916  CD  GLU A 921      39.514  58.054  21.899  1.00 41.44
ATOM    917  OE1 GLU A 921      40.583  58.228  22.581  1.00 41.44
ATOM    918  OE2 GLU A 921      39.465  58.066  20.642  1.00 41.44
ATOM    920  N   THR A 922      37.799  53.864  21.348  1.00 38.88
ATOM    921  CA  THR A 922      38.110  53.051  20.167  1.00 38.88
ATOM    922  C   THR A 922      36.981  52.136  19.842  1.00 38.88
ATOM    923  O   THR A 922      36.505  52.013  18.726  1.00 38.88
ATOM    924  CB  THR A 922      39.174  52.111  20.500  1.00 40.90
ATOM    925  OG1 THR A 922      39.068  51.846  21.908  1.00 40.90
ATOM    926  CG2 THR A 922      40.560  52.671  20.140  1.00 40.90
ATOM    929  N   ASP A 923      36.604  51.443  20.897  1.00 29.76
ATOM    930  CA  ASP A 923      35.585  50.420  20.901  1.00 29.76
ATOM    931  C   ASP A 923      34.964  50.486  22.309  1.00 29.76
ATOM    932  O   ASP A 923      35.466  49.896  23.271  1.00 29.76
ATOM    933  CB  ASP A 923      36.294  49.081  20.662  1.00100.00
ATOM    934  CG  ASP A 923      35.357  47.934  20.521  1.00100.00
ATOM    935  OD1 ASP A 923      35.131  47.241  21.517  1.00100.00
ATOM    936  OD2 ASP A 923      34.854  47.713  19.413  1.00100.00
ATOM    938  N   PRO A 924      33.906  51.274  22.472  1.00 69.79
ATOM    939  CA  PRO A 924      33.351  51.282  23.821  1.00 69.79
ATOM    940  C   PRO A 924      32.633  49.968  24.194  1.00 69.79
ATOM    941  O   PRO A 924      32.489  49.672  25.371  1.00 69.79
ATOM    942  CB  PRO A 924      32.449  52.516  23.822  1.00 55.89
ATOM    943  CG  PRO A 924      32.843  53.260  22.568  1.00 55.89
ATOM    944  CD  PRO A 924      33.238  52.242  21.601  1.00 55.89
ATOM    945  N   ALA A 925      32.206  49.183  23.199  1.00100.00
ATOM    946  CA  ALA A 925      31.555  47.887  23.453  1.00100.00
ATOM    947  C   ALA A 925      32.501  47.062  24.325  1.00100.00
ATOM    948  O   ALA A 925      32.137  46.651  25.428  1.00100.00
ATOM    949  CB  ALA A 925      31.278  47.156  22.146  1.00100.00
ATOM    951  N   PHE A 926      33.704  46.798  23.809  1.00 39.96
ATOM    952  CA  PHE A 926      34.714  46.108  24.576  1.00 39.96
ATOM    953  C   PHE A 926      34.808  46.862  25.859  1.00 39.96
ATOM    954  O   PHE A 926      34.279  46.468  26.851  1.00 39.96
ATOM    955  CB  PHE A 926      36.075  46.145  23.886  1.00 99.37
ATOM    956  CG  PHE A 926      37.128  45.350  24.602  1.00 99.37
ATOM    957  CD1 PHE A 926      37.270  43.990  24.365  1.00 99.37
ATOM    958  CD2 PHE A 926      37.940  45.950  25.560  1.00 99.37
ATOM    959  CE1 PHE A 926      38.192  43.248  25.071  1.00 99.37
ATOM    960  CE2 PHE A 926      38.861  45.217  26.265  1.00 99.37
ATOM    961  CZ  PHE A 926      38.987  43.863  26.023  1.00 99.37
ATOM    963  N   ALA A 927      35.470  47.996  25.823  1.00100.00
ATOM    964  CA  ALA A 927      35.628  48.798  27.018  1.00100.00
ATOM    965  C   ALA A 927      34.627  48.539  28.167  1.00100.00
ATOM    966  O   ALA A 927      35.030  48.490  29.328  1.00100.00
ATOM    967  CB  ALA A 927      35.611  50.250  26.619  1.00 37.88
ATOM    969  N   ILE A 928      33.343  48.348  27.845  1.00 71.50
ATOM    970  CA  ILE A 928      32.287  48.137  28.866  1.00 71.50
ATOM    971  C   ILE A 928      31.863  46.700  29.164  1.00 71.50
ATOM    972  O   ILE A 928      31.579  46.352  30.301  1.00 71.50
ATOM    973  CB  ILE A 928      30.987  48.939  28.510  1.00 96.87
ATOM    974  CG1 ILE A 928      30.326  49.467  29.787  1.00 96.87
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FIG. 6N

ATOM	975	CG2	ILE	A	928	30.008	48.051	27.748	1.00 96.87
ATOM	976	CD1	ILE	A	928	28.888	49.846	29.624	1.00 96.87
ATOM	978	N	ALA	A	929	31.793	45.881	28.130	1.00100.00
ATOM	979	CA	ALA	A	929	31.431	44.498	28.319	1.00100.00
ATOM	980	C	ALA	A	929	32.550	43.917	29.163	1.00100.00
ATOM	981	O	ALA	A	929	32.325	43.246	30.160	1.00100.00
ATOM	982	CB	ALA	A	929	31.367	43.810	26.982	1.00 31.88
ATOM	984	N	ASN	A	930	33.767	44.220	28.737	1.00 37.33
ATOM	985	CA	ASN	A	930	35.009	43.775	29.380	1.00 37.33
ATOM	986	C	ASN	A	930	35.326	44.575	30.614	1.00 37.33
ATOM	987	O	ASN	A	930	36.020	44.110	31.496	1.00 37.33
ATOM	988	CB	ASN	A	930	36.163	43.843	28.378	1.00 87.25
ATOM	989	CG	ASN	A	930	36.469	42.497	27.753	1.00 87.25
ATOM	990	OD1	ASN	A	930	37.485	41.865	28.062	1.00 87.25
ATOM	991	ND2	ASN	A	930	35.590	42.051	26.865	1.00 87.25
ATOM	995	N	SER	A	931	34.828	45.807	30.629	1.00 35.86
ATOM	996	CA	SER	A	931	34.968	46.734	31.740	1.00 35.86
ATOM	997	C	SER	A	931	36.347	47.321	32.044	1.00 35.86
ATOM	998	O	SER	A	931	36.779	47.344	33.211	1.00 35.86
ATOM	999	CB	SER	A	931	34.413	46.039	32.992	1.00 47.04
ATOM	1000	OG	SER	A	931	34.049	44.700	32.650	1.00 47.04
ATOM	1003	N	THR	A	932	37.030	47.813	31.024	1.00 77.19
ATOM	1004	CA	THR	A	932	38.346	48.398	31.249	1.00 77.19
ATOM	1005	C	THR	A	932	38.655	49.585	30.346	1.00 77.19
ATOM	1006	O	THR	A	932	38.224	49.632	29.198	1.00 77.19
ATOM	1007	CB	THR	A	932	39.453	47.353	31.056	1.00 99.17
ATOM	1008	OG1	THR	A	932	39.813	47.299	29.676	1.00 99.17
ATOM	1009	CG2	THR	A	932	38.980	45.991	31.492	1.00 99.17
ATOM	1012	N	ALA	A	933	39.376	50.554	30.891	1.00 37.14
ATOM	1013	CA	ALA	A	933	39.814	51.734	30.120	1.00 37.14
ATOM	1014	C	ALA	A	933	40.655	51.286	28.911	1.00 37.14
ATOM	1015	O	ALA	A	933	40.255	51.495	27.792	1.00 37.14
ATOM	1016	CB	ALA	A	933	40.625	52.743	31.046	1.00 2.00
ATOM	1018	N	SER	A	934	41.814	50.674	29.139	1.00 18.52
ATOM	1019	CA	SER	A	934	42.656	50.117	28.038	1.00 18.52
ATOM	1020	C	SER	A	934	42.578	48.537	27.897	1.00 18.52
ATOM	1021	O	SER	A	934	42.047	47.842	28.815	1.00 18.52
ATOM	1022	CB	SER	A	934	44.114	50.415	28.347	1.00 25.65
ATOM	1023	OG	SER	A	934	44.983	49.645	27.568	1.00 25.65
ATOM	1026	N	THR	A	935	43.162	48.023	26.794	1.00 63.20
ATOM	1027	CA	THR	A	935	43.338	46.574	26.529	1.00 63.20
ATOM	1028	C	THR	A	935	44.762	46.121	26.957	1.00 63.20
ATOM	1029	O	THR	A	935	45.084	44.947	26.871	1.00 63.20
ATOM	1030	CB	THR	A	935	43.298	46.147	25.069	1.00 29.40
ATOM	1031	OG1	THR	A	935	44.470	46.603	24.393	1.00 29.40
ATOM	1032	CG2	THR	A	935	42.095	46.590	24.385	1.00 29.40
ATOM	1035	N	LEU	A	936	45.616	47.065	27.349	1.00 6.64
ATOM	1036	CA	LEU	A	936	46.959	46.811	27.861	1.00 6.64
ATOM	1037	C	LEU	A	936	46.654	46.775	29.277	1.00 6.64
ATOM	1038	O	LEU	A	936	45.478	46.916	29.572	1.00 6.64
ATOM	1039	CB	LEU	A	936	47.962	47.919	27.602	1.00 2.00
ATOM	1040	CG	LEU	A	936	48.129	48.224	26.129	1.00 2.00
ATOM	1041	CD1	LEU	A	936	48.725	49.731	25.993	1.00 2.00
ATOM	1042	CD2	LEU	A	936	48.953	47.147	25.523	1.00 2.00
ATOM	1044	N	SER	A	937	47.638	46.528	30.129	1.00 38.75
ATOM	1045	CA	SER	A	937	47.437	46.434	31.555	1.00 38.75
ATOM	1046	C	SER	A	937	48.615	47.041	32.342	1.00 38.75

FIG. 60

ATOM	1047	O	SER	A	937	49.664	47.405	31.785	1.00	38.75
ATOM	1048	CB	SER	A	937	47.257	44.979	31.954	1.00	80.09
ATOM	1049	OG	SER	A	937	48.471	44.274	31.851	1.00	80.09
ATOM	1052	N	SER	A	938	48.441	47.158	33.646	1.00	54.88
ATOM	1053	CA	SER	A	938	49.489	47.699	34.441	1.00	54.88
ATOM	1054	C	SER	A	938	50.807	47.155	33.941	1.00	54.88
ATOM	1055	O	SER	A	938	51.696	47.907	33.571	1.00	54.88
ATOM	1056	CB	SER	A	938	49.295	47.312	35.887	1.00	69.11
ATOM	1057	OG	SER	A	938	50.397	47.773	36.631	1.00	69.11
ATOM	1060	N	GLN	A	939	50.906	45.831	33.902	1.00	55.81
ATOM	1061	CA	GLN	A	939	52.106	45.148	33.492	1.00	55.81
ATOM	1062	C	GLN	A	939	52.644	45.445	32.132	1.00	55.81
ATOM	1063	O	GLN	A	939	53.750	45.896	32.027	1.00	55.81
ATOM	1064	CB	GLN	A	939	51.924	43.650	33.615	1.00	74.76
ATOM	1065	CG	GLN	A	939	52.012	43.126	35.014	1.00	74.76
ATOM	1066	CD	GLN	A	939	53.409	42.973	35.514	1.00	74.76
ATOM	1067	OE1	GLN	A	939	54.238	42.296	34.906	1.00	74.76
ATOM	1068	NE2	GLN	A	939	53.684	43.597	36.648	1.00	74.76
ATOM	1072	N	GLN	A	940	51.899	45.176	31.069	1.00	26.74
ATOM	1073	CA	GLN	A	940	52.446	45.439	29.736	1.00	26.74
ATOM	1074	C	GLN	A	940	52.963	46.884	29.791	1.00	26.74
ATOM	1075	O	GLN	A	940	53.929	47.302	29.115	1.00	26.74
ATOM	1076	CB	GLN	A	940	51.405	45.313	28.639	1.00	43.63
ATOM	1077	CG	GLN	A	940	51.815	46.080	27.393	1.00	43.63
ATOM	1078	CD	GLN	A	940	52.444	45.214	26.267	1.00	43.63
ATOM	1079	OE1	GLN	A	940	51.734	44.544	25.479	1.00	43.63
ATOM	1080	NE2	GLN	A	940	53.756	45.236	26.183	1.00	43.63
ATOM	1084	N	LEU	A	941	52.300	47.595	30.698	1.00	30.59
ATOM	1085	CA	LEU	A	941	52.514	48.989	30.932	1.00	30.59
ATOM	1086	C	LEU	A	941	53.800	49.234	31.599	1.00	30.59
ATOM	1087	O	LEU	A	941	54.611	49.971	31.068	1.00	30.59
ATOM	1088	CB	LEU	A	941	51.334	49.521	31.709	1.00	27.00
ATOM	1089	CG	LEU	A	941	50.344	50.390	30.959	1.00	27.00
ATOM	1090	CD1	LEU	A	941	50.253	51.655	31.777	1.00	27.00
ATOM	1091	CD2	LEU	A	941	50.770	50.642	29.576	1.00	27.00
ATOM	1093	N	LEU	A	942	53.992	48.683	32.768	1.00	26.63
ATOM	1094	CA	LEU	A	942	55.284	48.801	33.427	1.00	26.63
ATOM	1095	C	LEU	A	942	56.433	48.144	32.573	1.00	26.63
ATOM	1096	O	LEU	A	942	57.616	48.326	32.850	1.00	26.63
ATOM	1097	CB	LEU	A	942	55.208	48.083	34.741	1.00	3.59
ATOM	1098	CG	LEU	A	942	55.275	49.016	35.906	1.00	3.59
ATOM	1099	CD1	LEU	A	942	55.141	48.265	37.321	1.00	3.59
ATOM	1100	CD2	LEU	A	942	56.635	49.823	35.675	1.00	3.59
ATOM	1102	N	HIS	A	943	56.084	47.359	31.562	1.00	54.79
ATOM	1103	CA	HIS	A	943	57.101	46.756	30.741	1.00	54.79
ATOM	1104	C	HIS	A	943	57.531	47.932	29.905	1.00	54.79
ATOM	1105	O	HIS	A	943	58.389	48.665	30.324	1.00	54.79
ATOM	1106	CB	HIS	A	943	56.530	45.638	29.852	1.00	38.35
ATOM	1107	CG	HIS	A	943	56.799	44.246	30.345	1.00	38.35
ATOM	1108	ND1	HIS	A	943	56.846	43.914	31.682	1.00	38.35
ATOM	1109	CD2	HIS	A	943	56.988	43.092	29.671	1.00	38.35
ATOM	1110	CE1	HIS	A	943	57.050	42.619	31.812	1.00	38.35
ATOM	1111	NE2	HIS	A	943	57.143	42.096	30.603	1.00	38.35
ATOM	1115	N	PHE	A	944	56.905	48.115	28.741	1.00	4.19
ATOM	1116	CA	PHE	A	944	57.172	49.217	27.780	1.00	4.19
ATOM	1117	C	PHE	A	944	58.218	50.257	28.412	1.00	4.19
ATOM	1118	O	PHE	A	944	59.278	50.592	27.781	1.00	4.19

FIG. 6P

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ATOM   1119  CB  PHE A 944      55.878  49.913  27.509  1.00 28.23
ATOM   1120  CG  PHE A 944      55.036  49.255  26.489  1.00 28.23
ATOM   1121  CD1 PHE A 944      53.632  49.319  26.610  1.00 28.23
ATOM   1122  CD2 PHE A 944      55.605  48.780  25.336  1.00 28.23
ATOM   1123  CE1 PHE A 944      52.813  48.958  25.614  1.00 28.23
ATOM   1124  CE2 PHE A 944      54.769  48.399  24.289  1.00 28.23
ATOM   1125  CZ  PHE A 944      53.342  48.504  24.452  1.00 28.23
ATOM   1127  N   ALA A 945      57.874  50.702  29.637  1.00 24.23
ATOM   1128  CA  ALA A 945      58.742  51.520  30.434  1.00 24.23
ATOM   1129  C   ALA A 945      59.943  50.648  30.375  1.00 24.23
ATOM   1130  O   ALA A 945      60.623  50.707  29.408  1.00 24.23
ATOM   1131  CB  ALA A 945      58.270  51.631  31.839  1.00 16.89
ATOM   1133  N   ALA A 946      60.153  49.775  31.366  1.00 23.93
ATOM   1134  CA  ALA A 946      61.327  48.819  31.493  1.00 23.93
ATOM   1135  C   ALA A 946      62.279  48.525  30.320  1.00 23.93
ATOM   1136  O   ALA A 946      63.460  48.674  30.432  1.00 23.93
ATOM   1137  CB  ALA A 946      60.834  47.495  32.054  1.00 76.24
ATOM   1139  N   ASP A 947      61.796  48.078  29.188  1.00  9.63
ATOM   1140  CA  ASP A 947      62.727  47.858  28.131  1.00  9.63
ATOM   1141  C   ASP A 947      63.169  49.132  27.456  1.00  9.63
ATOM   1142  O   ASP A 947      63.604  49.093  26.290  1.00  9.63
ATOM   1143  CB  ASP A 947      62.145  46.880  27.114  1.00 90.89
ATOM   1144  CG  ASP A 947      61.065  47.493  26.259  1.00 90.89
ATOM   1145  OD1 ASP A 947      60.143  46.747  25.854  1.00 90.89
ATOM   1146  OD2 ASP A 947      61.128  48.707  25.978  1.00 90.89
ATOM   1148  N   VAL A 948      63.024  50.287  28.098  1.00 60.29
ATOM   1149  CA  VAL A 948      63.435  51.532  27.459  1.00 60.29
ATOM   1150  C   VAL A 948      64.572  51.963  28.376  1.00 60.29
ATOM   1151  O   VAL A 948      65.604  52.405  27.907  1.00 60.29
ATOM   1152  CB  VAL A 948      62.213  52.606  27.324  1.00  2.00
ATOM   1153  CG1 VAL A 948      62.752  54.133  26.901  1.00  2.00
ATOM   1154  CG2 VAL A 948      61.348  52.297  26.209  1.00  2.00
ATOM   1156  N   ALA A 949      64.402  51.773  29.686  1.00 12.91
ATOM   1157  CA  ALA A 949      65.448  52.097  30.677  1.00 12.91
ATOM   1158  C   ALA A 949      66.681  51.382  30.188  1.00 12.91
ATOM   1159  O   ALA A 949      67.733  52.000  29.956  1.00 12.91
ATOM   1160  CB  ALA A 949      65.135  51.617  32.017  1.00  2.00
ATOM   1162  N   ARG A 950      66.484  50.078  30.000  1.00 22.64
ATOM   1163  CA  ARG A 950      67.422  49.105  29.537  1.00 22.64
ATOM   1164  C   ARG A 950      68.106  49.588  28.340  1.00 22.64
ATOM   1165  O   ARG A 950      69.275  49.681  28.386  1.00 22.64
ATOM   1166  CB  ARG A 950      66.702  47.783  29.233  1.00 87.27
ATOM   1167  CG  ARG A 950      67.146  46.606  30.102  1.00 87.27
ATOM   1168  CD  ARG A 950      66.806  45.233  29.493  1.00 87.27
ATOM   1169  NE  ARG A 950      65.466  45.208  28.912  1.00 87.27
ATOM   1170  CZ  ARG A 950      64.341  44.977  29.580  1.00 87.27
ATOM   1171  NH1 ARG A 950      64.357  44.746  30.879  1.00 87.27
ATOM   1172  NH2 ARG A 950      63.188  45.019  28.941  1.00 87.27
ATOM   1179  N   GLY A 951      67.435  49.846  27.241  1.00 33.31
ATOM   1180  CA  GLY A 951      68.177  50.360  26.102  1.00 33.31
ATOM   1181  C   GLY A 951      68.720  51.768  26.462  1.00 33.31
ATOM   1182  O   GLY A 951      69.514  52.379  25.745  1.00 33.31
ATOM   1184  N   MET A 952      68.277  52.318  27.588  1.00 48.02
ATOM   1185  CA  MET A 952      68.774  53.615  27.949  1.00 48.02
ATOM   1186  C   MET A 952      70.030  53.440  28.759  1.00 48.02
ATOM   1187  O   MET A 952      70.861  54.316  28.719  1.00 48.02
ATOM   1188  CB  MET A 952      67.721  54.442  28.720  1.00 58.75
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FIG. 6Q

ATOM	1189	CG	MET	A	952	67.277	55.792	28.089	1.00	58.75
ATOM	1190	SD	MET	A	952	67.797	56.265	26.390	1.00	58.75
ATOM	1191	CE	MET	A	952	69.079	57.471	26.826	1.00	58.75
ATOM	1193	N	ASP	A	953	70.145	52.325	29.494	1.00	30.83
ATOM	1194	CA	ASP	A	953	71.299	51.942	30.317	1.00	30.83
ATOM	1195	C	ASP	A	953	72.393	51.689	29.346	1.00	30.83
ATOM	1196	O	ASP	A	953	73.521	52.078	29.523	1.00	30.83
ATOM	1197	CB	ASP	A	953	71.084	50.617	30.955	1.00	30.69
ATOM	1198	CG	ASP	A	953	71.512	50.589	32.381	1.00	30.69
ATOM	1199	OD1	ASP	A	953	71.504	51.661	32.997	1.00	30.69
ATOM	1200	OD2	ASP	A	953	71.838	49.485	32.907	1.00	30.69
ATOM	1202	N	TYR	A	954	72.031	50.999	28.292	1.00	19.34
ATOM	1203	CA	TYR	A	954	72.952	50.630	27.239	1.00	19.34
ATOM	1204	C	TYR	A	954	73.559	51.896	26.762	1.00	19.34
ATOM	1205	O	TYR	A	954	74.529	52.327	27.362	1.00	19.34
ATOM	1206	CB	TYR	A	954	72.236	49.887	26.117	1.00	37.26
ATOM	1207	CG	TYR	A	954	73.181	49.115	25.244	1.00	37.26
ATOM	1208	CD1	TYR	A	954	74.158	48.238	25.784	1.00	37.26
ATOM	1209	CD2	TYR	A	954	73.149	49.300	23.871	1.00	37.26
ATOM	1210	CE1	TYR	A	954	75.072	47.594	24.942	1.00	37.26
ATOM	1211	CE2	TYR	A	954	74.042	48.676	23.041	1.00	37.26
ATOM	1212	CZ	TYR	A	954	74.993	47.843	23.568	1.00	37.26
ATOM	1213	OH	TYR	A	954	75.859	47.367	22.645	1.00	37.26
ATOM	1216	N	LEU	A	955	72.967	52.501	25.722	1.00	49.71
ATOM	1217	CA	LEU	A	955	73.404	53.781	25.150	1.00	49.71
ATOM	1218	C	LEU	A	955	73.854	54.641	26.293	1.00	49.71
ATOM	1219	O	LEU	A	955	74.950	55.109	26.279	1.00	49.71
ATOM	1220	CB	LEU	A	955	72.272	54.530	24.439	1.00	17.74
ATOM	1221	CG	LEU	A	955	71.456	53.937	23.292	1.00	17.74
ATOM	1222	CD1	LEU	A	955	69.972	54.493	23.397	1.00	17.74
ATOM	1223	CD2	LEU	A	955	71.989	54.345	21.914	1.00	17.74
ATOM	1225	N	SER	A	956	73.012	54.840	27.293	1.00	34.64
ATOM	1226	CA	SER	A	956	73.430	55.663	28.404	1.00	34.64
ATOM	1227	C	SER	A	956	74.843	55.360	28.778	1.00	34.64
ATOM	1228	O	SER	A	956	75.701	56.218	28.579	1.00	34.64
ATOM	1229	CB	SER	A	956	72.561	55.495	29.622	1.00	37.38
ATOM	1230	OG	SER	A	956	73.071	56.228	30.699	1.00	37.38
ATOM	1233	N	GLN	A	957	75.134	54.188	29.321	1.00	33.59
ATOM	1234	CA	GLN	A	957	76.511	53.895	29.680	1.00	33.59
ATOM	1235	C	GLN	A	957	77.379	53.837	28.410	1.00	33.59
ATOM	1236	O	GLN	A	957	77.719	52.798	27.943	1.00	33.59
ATOM	1237	CB	GLN	A	957	76.583	52.568	30.455	1.00	42.10
ATOM	1238	CG	GLN	A	957	76.621	52.721	32.002	1.00	42.10
ATOM	1239	CD	GLN	A	957	77.483	53.951	32.500	1.00	42.10
ATOM	1240	OE1	GLN	A	957	78.321	54.499	31.739	1.00	42.10
ATOM	1241	NE2	GLN	A	957	77.274	54.367	33.780	1.00	42.10
ATOM	1245	N	LYS	A	958	77.739	54.952	27.823	1.00	99.18
ATOM	1246	CA	LYS	A	958	78.543	54.854	26.620	1.00	99.18
ATOM	1247	C	LYS	A	958	78.688	56.227	26.039	1.00	99.18
ATOM	1248	O	LYS	A	958	79.111	56.370	24.897	1.00	99.18
ATOM	1249	CB	LYS	A	958	77.880	53.934	25.586	1.00	99.74
ATOM	1250	CG	LYS	A	958	78.545	52.582	25.404	1.00	99.74
ATOM	1251	CD	LYS	A	958	77.830	51.738	24.360	1.00	99.74
ATOM	1252	CE	LYS	A	958	77.997	50.238	24.629	1.00	99.74
ATOM	1253	NZ	LYS	A	958	78.459	49.456	23.434	1.00	99.74
ATOM	1258	N	GLN	A	959	78.327	57.233	26.832	1.00	73.45
ATOM	1259	CA	GLN	A	959	78.423	58.615	26.402	1.00	73.45

FIG. 6R

```
ATOM   1260  C   GLN A 959      77.378  58.947  25.376  1.00 73.45
ATOM   1261  O   GLN A 959      77.493  59.970  24.702  1.00 73.45
ATOM   1262  CB  GLN A 959      79.785  58.882  25.784  1.00 19.35
ATOM   1263  CG  GLN A 959      80.899  58.069  26.399  1.00 19.35
ATOM   1264  CD  GLN A 959      80.957  58.449  27.805  1.00 19.35
ATOM   1265  OE1 GLN A 959      80.252  59.453  28.221  1.00 19.35
ATOM   1266  NE2 GLN A 959      81.763  57.708  28.610  1.00 19.35
ATOM   1270  N   PHE A 960      76.376  58.075  25.242  1.00 36.08
ATOM   1271  CA  PHE A 960      75.312  58.292  24.262  1.00 36.08
ATOM   1272  C   PHE A 960      74.223  59.102  24.956  1.00 36.08
ATOM   1273  O   PHE A 960      73.754  58.762  26.078  1.00 36.08
ATOM   1274  CB  PHE A 960      74.810  56.957  23.718  1.00 85.11
ATOM   1275  CG  PHE A 960      75.670  56.407  22.614  1.00 85.11
ATOM   1276  CD1 PHE A 960      76.531  55.349  22.839  1.00 85.11
ATOM   1277  CD2 PHE A 960      75.656  56.981  21.350  1.00 85.11
ATOM   1278  CE1 PHE A 960      77.361  54.879  21.822  1.00 85.11
ATOM   1279  CE2 PHE A 960      76.493  56.505  20.330  1.00 85.11
ATOM   1280  CZ  PHE A 960      77.338  55.461  20.572  1.00 85.11
ATOM   1282  N   ILE A 961      73.918  60.227  24.300  1.00 30.22
ATOM   1283  CA  ILE A 961      72.939  61.196  24.749  1.00 30.22
ATOM   1284  C   ILE A 961      71.858  61.213  23.713  1.00 30.22
ATOM   1285  O   ILE A 961      72.112  61.420  22.545  1.00 30.22
ATOM   1286  CB  ILE A 961      73.536  62.578  24.911  1.00 71.39
ATOM   1287  CG1 ILE A 961      74.693  62.526  25.899  1.00 71.39
ATOM   1288  CG2 ILE A 961      72.488  63.518  25.442  1.00 71.39
ATOM   1289  CD1 ILE A 961      75.888  63.302  25.476  1.00 71.39
ATOM   1291  N   HIS A 962      70.627  61.034  24.158  1.00 80.58
ATOM   1292  CA  HIS A 962      69.524  60.924  23.236  1.00 80.58
ATOM   1293  C   HIS A 962      68.798  62.196  22.692  1.00 80.58
ATOM   1294  O   HIS A 962      69.179  62.676  21.629  1.00 80.58
ATOM   1295  CB  HIS A 962      68.584  59.904  23.855  1.00 39.42
ATOM   1296  CG  HIS A 962      67.415  59.585  23.008  1.00 39.42
ATOM   1297  ND1 HIS A 962      67.142  58.316  22.575  1.00 39.42
ATOM   1298  CD2 HIS A 962      66.450  60.378  22.499  1.00 39.42
ATOM   1299  CE1 HIS A 962      66.052  58.335  21.832  1.00 39.42
ATOM   1300  NE2 HIS A 962      65.617  59.580  21.772  1.00 39.42
ATOM   1304  N   ARG A 963      67.745  62.694  23.367  1.00 25.62
ATOM   1305  CA  ARG A 963      67.008  63.920  22.979  1.00 25.62
ATOM   1306  C   ARG A 963      65.777  63.852  22.084  1.00 25.62
ATOM   1307  O   ARG A 963      65.762  64.331  20.941  1.00 25.62
ATOM   1308  CB  ARG A 963      67.977  64.955  22.380  1.00 98.75
ATOM   1309  CG  ARG A 963      69.318  65.061  23.081  1.00 98.75
ATOM   1310  CD  ARG A 963      70.230  66.016  22.356  1.00 98.75
ATOM   1311  NE  ARG A 963      70.718  65.501  21.087  1.00 98.75
ATOM   1312  CZ  ARG A 963      70.212  65.832  19.911  1.00 98.75
ATOM   1313  NH1 ARG A 963      69.200  66.680  19.852  1.00 98.75
ATOM   1314  NH2 ARG A 963      70.717  65.321  18.801  1.00 98.75
ATOM   1321  N   ASN A 964      64.738  63.276  22.661  1.00 47.91
ATOM   1322  CA  ASN A 964      63.442  63.070  22.035  1.00 47.91
ATOM   1323  C   ASN A 964      63.235  61.618  22.246  1.00 47.91
ATOM   1324  O   ASN A 964      63.068  60.856  21.302  1.00 47.91
ATOM   1325  CB  ASN A 964      63.453  63.377  20.538  1.00 84.77
ATOM   1326  CG  ASN A 964      62.453  64.459  20.153  1.00 84.77
ATOM   1327  OD1 ASN A 964      61.509  64.768  20.902  1.00 84.77
ATOM   1328  ND2 ASN A 964      62.653  65.039  18.977  1.00 84.77
ATOM   1332  N   LEU A 965      63.366  61.249  23.509  1.00 96.70
ATOM   1333  CA  LEU A 965      63.148  59.897  23.937  1.00 96.70
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FIG. 6S

ATOM	1334	C	LEU	A	965	61.836	60.220	24.659	1.00	96.70
ATOM	1335	O	LEU	A	965	61.784	60.527	25.833	1.00	96.70
ATOM	1336	CB	LEU	A	965	64.352	59.382	24.805	1.00	17.46
ATOM	1337	CG	LEU	A	965	64.456	58.589	26.099	1.00	17.46
ATOM	1338	CD1	LEU	A	965	65.774	58.784	26.891	1.00	17.46
ATOM	1339	CD2	LEU	A	965	63.423	59.114	26.967	1.00	17.46
ATOM	1341	N	ALA	A	966	60.794	60.283	23.833	1.00	71.46
ATOM	1342	CA	ALA	A	966	59.408	60.534	24.219	1.00	71.46
ATOM	1343	C	ALA	A	966	58.601	59.518	23.395	1.00	71.46
ATOM	1344	O	ALA	A	966	59.009	59.122	22.314	1.00	71.46
ATOM	1345	CB	ALA	A	966	59.005	61.933	23.885	1.00	62.29
ATOM	1347	N	ALA	A	967	57.457	59.105	23.908	1.00	34.40
ATOM	1348	CA	ALA	A	967	56.641	58.086	23.249	1.00	34.40
ATOM	1349	C	ALA	A	967	56.585	58.066	21.726	1.00	34.40
ATOM	1350	O	ALA	A	967	56.689	57.011	21.106	1.00	34.40
ATOM	1351	CB	ALA	A	967	55.236	58.088	23.807	1.00	31.96
ATOM	1353	N	ARG	A	968	56.462	59.208	21.094	1.00	9.59
ATOM	1354	CA	ARG	A	968	56.309	59.113	19.678	1.00	9.59
ATOM	1355	C	ARG	A	968	57.467	58.532	19.054	1.00	9.59
ATOM	1356	O	ARG	A	968	57.335	58.106	17.930	1.00	9.59
ATOM	1357	CB	ARG	A	968	55.960	60.480	19.013	1.00	12.36
ATOM	1358	CG	ARG	A	968	56.480	61.806	19.751	1.00	12.36
ATOM	1359	CD	ARG	A	968	56.426	62.907	18.727	1.00	12.36
ATOM	1360	NE	ARG	A	968	57.453	63.898	18.879	1.00	12.36
ATOM	1361	CZ	ARG	A	968	57.608	64.568	19.994	1.00	12.36
ATOM	1362	NH1	ARG	A	968	56.746	64.307	20.994	1.00	12.36
ATOM	1363	NH2	ARG	A	968	58.718	65.297	20.206	1.00	12.36
ATOM	1370	N	ASN	A	969	58.611	58.550	19.735	1.00	56.22
ATOM	1371	CA	ASN	A	969	59.878	58.043	19.179	1.00	56.22
ATOM	1372	C	ASN	A	969	60.309	56.672	19.730	1.00	56.22
ATOM	1373	O	ASN	A	969	61.472	56.327	19.673	1.00	56.22
ATOM	1374	CB	ASN	A	969	61.011	59.053	19.444	1.00	99.68
ATOM	1375	CG	ASN	A	969	60.674	60.482	18.998	1.00	99.68
ATOM	1376	OD1	ASN	A	969	60.213	61.303	19.787	1.00	99.68
ATOM	1377	ND2	ASN	A	969	60.926	60.780	17.732	1.00	99.68
ATOM	1381	N	ILE	A	970	59.351	55.935	20.288	1.00	10.68
ATOM	1382	CA	ILE	A	970	59.507	54.683	20.853	1.00	10.68
ATOM	1383	C	ILE	A	970	58.651	53.708	20.079	1.00	10.68
ATOM	1384	O	ILE	A	970	57.450	53.865	20.060	1.00	10.68
ATOM	1385	CB	ILE	A	970	59.003	54.602	22.168	1.00	11.62
ATOM	1386	CG1	ILE	A	970	59.808	55.496	23.084	1.00	11.62
ATOM	1387	CG2	ILE	A	970	59.191	53.056	22.620	1.00	11.62
ATOM	1388	CD1	ILE	A	970	61.263	55.730	22.600	1.00	11.62
ATOM	1390	N	LEU	A	971	59.250	52.676	19.496	1.00	31.69
ATOM	1391	CA	LEU	A	971	58.518	51.699	18.733	1.00	31.69
ATOM	1392	C	LEU	A	971	58.148	50.357	19.369	1.00	31.69
ATOM	1393	O	LEU	A	971	58.938	49.792	20.148	1.00	31.69
ATOM	1394	CB	LEU	A	971	59.308	51.333	17.535	1.00	17.23
ATOM	1395	CG	LEU	A	971	59.702	52.411	16.632	1.00	17.23
ATOM	1396	CD1	LEU	A	971	60.981	51.973	16.005	1.00	17.23
ATOM	1397	CD2	LEU	A	971	58.629	52.642	15.646	1.00	17.23
ATOM	1399	N	VAL	A	972	56.953	49.832	19.017	1.00	20.91
ATOM	1400	CA	VAL	A	972	56.655	48.486	19.475	1.00	20.91
ATOM	1401	C	VAL	A	972	56.862	47.491	18.389	1.00	20.91
ATOM	1402	O	VAL	A	972	56.022	47.375	17.523	1.00	20.91
ATOM	1403	CB	VAL	A	972	55.344	48.349	19.953	1.00	9.13
ATOM	1404	CG1	VAL	A	972	55.362	47.291	21.081	1.00	9.13

FIG. 6T

ATOM	1405	CG2	VAL	A	972	54.797	49.894	20.467	1.00	9.13
ATOM	1407	N	GLY	A	973	58.077	46.873	18.414	1.00	32.46
ATOM	1408	CA	GLY	A	973	58.514	45.851	17.466	1.00	32.46
ATOM	1409	C	GLY	A	973	58.012	44.434	17.814	1.00	32.46
ATOM	1410	O	GLY	A	973	57.324	44.254	18.816	1.00	32.46
ATOM	1412	N	GLU	A	974	58.393	43.403	17.055	1.00	22.44
ATOM	1413	CA	GLU	A	974	57.846	42.109	17.351	1.00	22.44
ATOM	1414	C	GLU	A	974	57.902	41.725	18.793	1.00	22.44
ATOM	1415	O	GLU	A	974	58.809	42.041	19.510	1.00	22.44
ATOM	1416	CB	GLU	A	974	58.364	41.035	16.394	1.00	65.78
ATOM	1417	CG	GLU	A	974	57.385	40.798	15.138	1.00	65.78
ATOM	1418	CD	GLU	A	974	55.821	40.585	15.469	1.00	65.78
ATOM	1419	OE1	GLU	A	974	55.398	40.463	16.656	1.00	65.78
ATOM	1420	OE2	GLU	A	974	55.005	40.540	14.512	1.00	65.78
ATOM	1422	N	ASN	A	975	56.767	41.210	19.246	1.00	22.08
ATOM	1423	CA	ASN	A	975	56.540	40.717	20.627	1.00	22.08
ATOM	1424	C	ASN	A	975	56.037	41.756	21.638	1.00	22.08
ATOM	1425	O	ASN	A	975	55.968	41.482	22.844	1.00	22.08
ATOM	1426	CB	ASN	A	975	57.810	40.016	21.140	1.00	99.25
ATOM	1427	CG	ASN	A	975	58.074	38.679	20.438	1.00	99.25
ATOM	1428	OD1	ASN	A	975	58.836	37.859	20.929	1.00	99.25
ATOM	1429	ND2	ASN	A	975	57.446	38.465	19.292	1.00	99.25
ATOM	1433	N	TYR	A	976	55.656	42.932	21.134	1.00	30.29
ATOM	1434	CA	TYR	A	976	55.204	44.013	21.972	1.00	30.29
ATOM	1435	C	TYR	A	976	56.427	44.631	22.697	1.00	30.29
ATOM	1436	O	TYR	A	976	56.331	45.214	23.759	1.00	30.29
ATOM	1437	CB	TYR	A	976	54.157	43.463	22.893	1.00	71.60
ATOM	1438	CG	TYR	A	976	53.001	42.961	22.089	1.00	71.60
ATOM	1439	CD1	TYR	A	976	52.698	41.611	22.036	1.00	71.60
ATOM	1440	CD2	TYR	A	976	52.229	43.840	21.339	1.00	71.60
ATOM	1441	CE1	TYR	A	976	51.652	41.145	21.243	1.00	71.60
ATOM	1442	CE2	TYR	A	976	51.181	43.390	20.547	1.00	71.60
ATOM	1443	CZ	TYR	A	976	50.895	42.043	20.491	1.00	71.60
ATOM	1444	OH	TYR	A	976	49.905	41.588	19.655	1.00	71.60
ATOM	1447	N	VAL	A	977	57.569	44.513	22.047	1.00	35.58
ATOM	1448	CA	VAL	A	977	58.837	44.988	22.597	1.00	35.58
ATOM	1449	C	VAL	A	977	59.247	46.367	22.101	1.00	35.58
ATOM	1450	O	VAL	A	977	59.495	46.616	20.903	1.00	35.58
ATOM	1451	CB	VAL	A	977	59.994	43.975	22.316	1.00	54.29
ATOM	1452	CG1	VAL	A	977	61.110	44.134	23.340	1.00	54.29
ATOM	1453	CG2	VAL	A	977	59.418	42.533	22.339	1.00	54.29
ATOM	1455	N	ALA	A	978	59.355	47.233	23.082	1.00	36.83
ATOM	1456	CA	ALA	A	978	59.628	48.594	22.857	1.00	36.83
ATOM	1457	C	ALA	A	978	61.086	49.005	22.550	1.00	36.83
ATOM	1458	O	ALA	A	978	61.937	48.823	23.380	1.00	36.83
ATOM	1459	CB	ALA	A	978	59.142	49.265	24.019	1.00	27.14
ATOM	1461	N	LYS	A	979	61.368	49.570	21.374	1.00	42.93
ATOM	1462	CA	LYS	A	979	62.704	50.023	21.063	1.00	42.93
ATOM	1463	C	LYS	A	979	63.002	51.530	20.907	1.00	42.93
ATOM	1464	O	LYS	A	979	62.175	52.352	20.414	1.00	42.93
ATOM	1465	CB	LYS	A	979	63.190	49.433	19.798	1.00	32.23
ATOM	1466	CG	LYS	A	979	62.273	48.708	19.039	1.00	32.23
ATOM	1467	CD	LYS	A	979	62.556	47.230	19.416	1.00	32.23
ATOM	1468	CE	LYS	A	979	63.156	46.356	18.275	1.00	32.23
ATOM	1469	NZ	LYS	A	979	63.744	45.144	18.883	1.00	32.23
ATOM	1474	N	ILE	A	980	64.233	51.887	21.275	1.00	2.00
ATOM	1475	CA	ILE	A	980	64.639	53.265	21.099	1.00	2.00

FIG. 6U

ATOM	1476	C	ILE	A	980	65.044	53.446	19.649	1.00 2.00
ATOM	1477	O	ILE	A	980	65.191	52.445	18.913	1.00 2.00
ATOM	1478	CB	ILE	A	980	65.717	53.649	22.013	1.00 22.25
ATOM	1479	CG1	ILE	A	980	65.318	53.372	23.463	1.00 22.25
ATOM	1480	CG2	ILE	A	980	65.839	55.073	21.885	1.00 22.25
ATOM	1481	CD1	ILE	A	980	66.358	53.040	24.467	1.00 22.25
ATOM	1483	N	ALA	A	981	65.129	54.715	19.235	1.00 37.10
ATOM	1484	CA	ALA	A	981	65.489	55.166	17.870	1.00 37.10
ATOM	1485	C	ALA	A	981	65.426	56.684	17.652	1.00 37.10
ATOM	1486	O	ALA	A	981	64.905	57.454	18.494	1.00 37.10
ATOM	1487	CB	ALA	A	981	64.634	54.620	16.964	1.00 12.10
ATOM	1489	N	ASP	A	982	65.933	57.120	16.508	1.00 81.89
ATOM	1490	CA	ASP	A	982	65.907	58.525	16.186	1.00 81.89
ATOM	1491	C	ASP	A	982	66.821	59.190	17.201	1.00 81.89
ATOM	1492	O	ASP	A	982	66.877	60.416	17.342	1.00 81.89
ATOM	1493	CB	ASP	A	982	64.465	59.029	16.284	1.00 22.36
ATOM	1494	CG	ASP	A	982	64.352	60.357	16.999	1.00 22.36
ATOM	1495	OD1	ASP	A	982	64.517	61.390	16.281	1.00 22.36
ATOM	1496	OD2	ASP	A	982	64.112	60.353	18.252	1.00 22.36
ATOM	1498	N	PHE	A	983	67.540	58.353	17.922	1.00 90.03
ATOM	1499	CA	PHE	A	983	68.502	58.819	18.897	1.00 90.03
ATOM	1500	C	PHE	A	983	69.521	59.638	18.083	1.00 90.03
ATOM	1501	O	PHE	A	983	69.436	59.728	16.844	1.00 90.03
ATOM	1502	CB	PHE	A	983	69.205	57.599	19.489	1.00100.00
ATOM	1503	CG	PHE	A	983	69.417	56.489	18.475	1.00100.00
ATOM	1504	CD1	PHE	A	983	70.419	56.593	17.502	1.00100.00
ATOM	1505	CD2	PHE	A	983	68.567	55.387	18.435	1.00100.00
ATOM	1506	CE1	PHE	A	983	70.557	55.624	16.513	1.00100.00
ATOM	1507	CE2	PHE	A	983	68.704	54.418	17.449	1.00100.00
ATOM	1508	CZ	PHE	A	983	69.698	54.537	16.488	1.00100.00
ATOM	1510	N	GLY	A	984	70.493	60.226	18.770	1.00 59.78
ATOM	1511	CA	GLY	A	984	71.533	60.957	18.060	1.00 59.78
ATOM	1512	C	GLY	A	984	72.821	60.159	18.193	1.00 59.78
ATOM	1513	O	GLY	A	984	72.900	59.221	19.019	1.00 59.78
ATOM	1515	N	LEU	A	985	73.816	60.488	17.379	1.00 99.32
ATOM	1516	CA	LEU	A	985	75.094	59.791	17.454	1.00 99.32
ATOM	1517	C	LEU	A	985	75.886	60.603	18.440	1.00 99.32
ATOM	1518	O	LEU	A	985	77.068	60.348	18.669	1.00 99.32
ATOM	1519	CB	LEU	A	985	75.824	59.786	16.106	1.00100.00
ATOM	1520	CG	LEU	A	985	75.453	58.753	15.036	1.00100.00
ATOM	1521	CD1	LEU	A	985	74.707	57.590	15.651	1.00100.00
ATOM	1522	CD2	LEU	A	985	74.604	59.428	13.971	1.00100.00
ATOM	1524	N	SER	A	986	75.211	61.587	19.020	1.00 37.75
ATOM	1525	CA	SER	A	986	75.828	62.476	19.989	1.00 37.75
ATOM	1526	C	SER	A	986	76.413	61.806	21.210	1.00 37.75
ATOM	1527	O	SER	A	986	75.708	61.541	22.143	1.00 37.75
ATOM	1528	CB	SER	A	986	74.830	63.525	20.445	1.00 99.91
ATOM	1529	OG	SER	A	986	75.198	64.776	19.917	1.00 99.91
ATOM	1532	N	ARG	A	987	77.710	61.513	21.216	1.00 63.13
ATOM	1533	CA	ARG	A	987	78.285	60.910	22.407	1.00 63.13
ATOM	1534	C	ARG	A	987	79.243	61.904	22.979	1.00 63.13
ATOM	1535	O	ARG	A	987	80.058	62.476	22.270	1.00 63.13
ATOM	1536	CB	ARG	A	987	78.964	59.567	22.132	1.00 87.40
ATOM	1537	CG	ARG	A	987	79.870	59.529	20.947	1.00 87.40
ATOM	1538	CD	ARG	A	987	81.110	58.722	21.273	1.00 87.40
ATOM	1539	NE	ARG	A	987	80.807	57.654	22.217	1.00 87.40
ATOM	1540	CZ	ARG	A	987	80.782	56.366	21.898	1.00 87.40

FIG. 6V

ATOM	1541	NH1	ARG	A	987	81.042	55.981	20.658	1.00 87.40
ATOM	1542	NH2	ARG	A	987	80.506	55.463	22.824	1.00 87.40
ATOM	1549	N	GLY	A	988	79.090	62.096	24.282	1.00 28.62
ATOM	1550	CA	GLY	A	988	79.833	63.044	25.072	1.00 28.62
ATOM	1551	C	GLY	A	988	79.268	63.073	26.476	1.00 28.62
ATOM	1552	O	GLY	A	988	78.558	62.156	26.816	1.00 28.62
ATOM	1554	N	GLN	A	989	79.612	64.094	27.270	1.00 22.70
ATOM	1555	CA	GLN	A	989	79.214	64.322	28.682	1.00 22.70
ATOM	1556	C	GLN	A	989	78.188	65.518	28.775	1.00 22.70
ATOM	1557	O	GLN	A	989	77.534	65.676	29.785	1.00 22.70
ATOM	1558	CB	GLN	A	989	80.449	64.647	29.536	1.00 98.73
ATOM	1559	CG	GLN	A	989	80.240	64.572	31.049	1.00 98.73
ATOM	1560	CD	GLN	A	989	81.127	65.539	31.844	1.00 98.73
ATOM	1561	OE1	GLN	A	989	81.240	66.712	31.510	1.00 98.73
ATOM	1562	NE2	GLN	A	989	81.746	65.043	32.901	1.00 98.73
ATOM	1566	N	GLU	A	990	78.055	66.323	27.724	1.00 47.13
ATOM	1567	CA	GLU	A	990	77.173	67.478	27.725	1.00 47.13
ATOM	1568	C	GLU	A	990	77.106	67.842	26.251	1.00 47.13
ATOM	1569	O	GLU	A	990	78.116	67.765	25.565	1.00 47.13
ATOM	1570	CB	GLU	A	990	77.830	68.612	28.534	1.00 77.23
ATOM	1571	CG	GLU	A	990	76.950	69.834	28.830	1.00 77.23
ATOM	1572	CD	GLU	A	990	76.930	70.244	30.322	1.00 77.23
ATOM	1573	OE1	GLU	A	990	77.431	69.468	31.165	1.00 77.23
ATOM	1574	OE2	GLU	A	990	76.406	71.337	30.658	1.00 77.23
ATOM	1576	N	VAL	A	991	75.946	68.228	25.727	1.00 24.20
ATOM	1577	CA	VAL	A	991	75.831	68.569	24.274	1.00 24.20
ATOM	1578	C	VAL	A	991	75.272	69.989	24.073	1.00 24.20
ATOM	1579	O	VAL	A	991	75.089	70.682	25.017	1.00 24.20
ATOM	1580	CB	VAL	A	991	74.897	67.572	23.527	1.00 55.15
ATOM	1581	CG1	VAL	A	991	75.197	67.520	22.035	1.00 55.15
ATOM	1582	CG2	VAL	A	991	75.015	66.252	24.148	1.00 55.15
ATOM	1584	N	TYR	A	992	75.056	70.398	22.840	1.00 53.40
ATOM	1585	CA	TYR	A	992	74.514	71.693	22.545	1.00 53.40
ATOM	1586	C	TYR	A	992	73.954	71.659	21.140	1.00 53.40
ATOM	1587	O	TYR	A	992	74.678	71.455	20.177	1.00 53.40
ATOM	1588	CB	TYR	A	992	75.594	72.774	22.658	1.00 83.17
ATOM	1589	CG	TYR	A	992	75.167	74.067	22.018	1.00 83.17
ATOM	1590	CD1	TYR	A	992	74.337	74.950	22.688	1.00 83.17
ATOM	1591	CD2	TYR	A	992	75.452	74.316	20.694	1.00 83.17
ATOM	1592	CE1	TYR	A	992	73.796	76.025	22.047	1.00 83.17
ATOM	1593	CE2	TYR	A	992	74.919	75.380	20.053	1.00 83.17
ATOM	1594	CZ	TYR	A	992	74.090	76.230	20.726	1.00 83.17
ATOM	1595	OH	TYR	A	992	73.569	77.297	20.053	1.00 83.17
ATOM	1598	N	VAL	A	993	72.645	71.821	21.015	1.00100.00
ATOM	1599	CA	VAL	A	993	72.047	71.808	19.695	1.00100.00
ATOM	1600	C	VAL	A	993	70.897	72.813	19.594	1.00100.00
ATOM	1601	O	VAL	A	993	69.736	72.514	19.912	1.00100.00
ATOM	1602	CB	VAL	A	993	71.604	70.371	19.304	1.00 80.14
ATOM	1603	CG1	VAL	A	993	71.422	69.529	20.538	1.00 80.14
ATOM	1604	CG2	VAL	A	993	70.338	70.409	18.450	1.00 80.14
ATOM	1606	N	LYS	A	994	71.260	74.022	19.155	1.00 83.98
ATOM	1607	CA	LYS	A	994	70.329	75.125	18.980	1.00 83.98
ATOM	1608	C	LYS	A	994	69.729	74.959	17.615	1.00 83.98
ATOM	1609	O	LYS	A	994	70.421	74.538	16.688	1.00 83.98
ATOM	1610	CB	LYS	A	994	71.076	76.455	19.070	1.00100.00
ATOM	1611	CG	LYS	A	994	70.350	77.670	18.498	1.00100.00
ATOM	1612	CD	LYS	A	994	71.347	78.789	18.226	1.00100.00

FIG. 6W

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ATOM   1613  CE  LYS A 994      70.694  80.150  18.153  1.00100.00
ATOM   1614  NZ  LYS A 994      71.425  81.159  18.962  1.00100.00
ATOM   1615  N   LYS A 995      68.446  75.287  17.488  1.00 66.77
ATOM   1620  CA  LYS A 995      67.741  75.142  16.210  1.00 66.77
ATOM   1621  C   LYS A 995      68.023  73.749  15.591  1.00 66.77
ATOM   1622  O   LYS A 995      67.910  73.583  14.358  1.00 66.77
ATOM   1623  CB  LYS A 995      68.167  76.265  15.244  1.00100.00
ATOM   1624  OXT LYS A 995      68.354  72.815  16.355  1.00100.00
ATOM   1626  N   PRO A1001      61.032  69.682  22.189  1.00 23.57
ATOM   1627  CA  PRO A1001      59.754  69.092  22.679  1.00 23.57
ATOM   1628  C   PRO A1001      59.681  69.765  24.004  1.00 23.57
ATOM   1629  O   PRO A1001      59.857  69.162  25.026  1.00 23.57
ATOM   1630  CB  PRO A1001      59.964  67.607  22.863  1.00 82.24
ATOM   1631  CG  PRO A1001      61.529  67.446  22.804  1.00 82.24
ATOM   1632  CD  PRO A1001      62.179  68.812  22.494  1.00 82.24
ATOM   1635  N   VAL A1002      59.429  71.067  23.965  1.00 14.96
ATOM   1636  CA  VAL A1002      59.401  71.905  25.163  1.00 14.96
ATOM   1637  C   VAL A1002      58.731  71.247  26.277  1.00 14.96
ATOM   1638  O   VAL A1002      58.930  71.607  27.409  1.00 14.96
ATOM   1639  CB  VAL A1002      58.755  73.268  24.833  1.00 66.63
ATOM   1640  CG1 VAL A1002      57.691  73.065  23.764  1.00 66.63
ATOM   1641  CG2 VAL A1002      58.212  73.946  26.088  1.00 66.63
ATOM   1643  N   ARG A1003      57.913  70.256  25.990  1.00 36.10
ATOM   1644  CA  ARG A1003      57.188  69.580  27.054  1.00 36.10
ATOM   1645  C   ARG A1003      57.957  68.409  27.649  1.00 36.10
ATOM   1646  O   ARG A1003      57.762  68.012  28.773  1.00 36.10
ATOM   1647  CB  ARG A1003      55.829  69.195  26.507  1.00 97.10
ATOM   1648  CG  ARG A1003      55.381  70.237  25.495  1.00 97.10
ATOM   1649  CD  ARG A1003      53.974  70.007  25.036  1.00 97.10
ATOM   1650  NE  ARG A1003      53.022  70.432  26.045  1.00 97.10
ATOM   1651  CZ  ARG A1003      51.949  71.153  25.782  1.00 97.10
ATOM   1652  NH1 ARG A1003      51.699  71.527  24.544  1.00 97.10
ATOM   1653  NH2 ARG A1003      51.136  71.493  26.759  1.00 97.10
ATOM   1660  N   TRP A1004      58.902  67.934  26.865  1.00 31.39
ATOM   1661  CA  TRP A1004      59.799  66.858  27.231  1.00 31.39
ATOM   1662  C   TRP A1004      61.031  67.342  27.941  1.00 31.39
ATOM   1663  O   TRP A1004      61.431  66.841  28.992  1.00 31.39
ATOM   1664  CB  TRP A1004      60.117  66.113  25.981  1.00 37.57
ATOM   1665  CG  TRP A1004      59.058  65.128  25.860  1.00 37.57
ATOM   1666  CD1 TRP A1004      59.055  63.870  26.415  1.00 37.57
ATOM   1667  CD2 TRP A1004      57.758  65.324  25.323  1.00 37.57
ATOM   1668  NE1 TRP A1004      57.832  63.290  26.253  1.00 37.57
ATOM   1669  CE2 TRP A1004      57.011  64.149  25.594  1.00 37.57
ATOM   1670  CE3 TRP A1004      57.142  66.370  24.648  1.00 37.57
ATOM   1671  CZ2 TRP A1004      55.683  63.991  25.214  1.00 37.57
ATOM   1672  CZ3 TRP A1004      55.789  66.223  24.252  1.00 37.57
ATOM   1673  CH2 TRP A1004      55.087  65.041  24.541  1.00 37.57
ATOM   1676  N   MET A1005      61.556  68.426  27.391  1.00 10.72
ATOM   1677  CA  MET A1005      62.723  69.067  27.879  1.00 10.72
ATOM   1678  C   MET A1005      62.709  69.405  29.340  1.00 10.72
ATOM   1679  O   MET A1005      61.690  69.822  29.947  1.00 10.72
ATOM   1680  CB  MET A1005      62.983  70.254  27.003  1.00 63.30
ATOM   1681  CG  MET A1005      63.299  69.783  25.632  1.00 63.30
ATOM   1682  SD  MET A1005      63.194  71.078  24.467  1.00 63.30
ATOM   1683  CE  MET A1005      64.494  72.111  25.002  1.00 63.30
ATOM   1685  N   ALA A1006      63.873  69.180  29.939  1.00 13.71
ATOM   1686  CA  ALA A1006      64.092  69.541  31.343  1.00 13.71
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FIG. 6X

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ATOM   1687  C   ALA A1006      64.634  71.015  31.321  1.00 13.71
ATOM   1688  O   ALA A1006      64.885  71.575  30.254  1.00 13.71
ATOM   1689  CB  ALA A1006      65.114  68.618  31.976  1.00 44.23
ATOM   1691  N   ILE A1007      64.762  71.597  32.515  1.00 21.54
ATOM   1692  CA  ILE A1007      65.278  72.951  32.738  1.00 21.54
ATOM   1693  C   ILE A1007      66.586  73.324  31.943  1.00 21.54
ATOM   1694  O   ILE A1007      66.528  73.791  30.817  1.00 21.54
ATOM   1695  CB  ILE A1007      65.482  73.137  34.300  1.00 20.90
ATOM   1696  CG1 ILE A1007      66.672  72.188  34.830  1.00 20.90
ATOM   1697  CG2 ILE A1007      64.088  72.800  35.034  1.00 20.90
ATOM   1698  CD1 ILE A1007      67.395  72.474  36.237  1.00 20.90
ATOM   1700  N   GLU A1008      67.752  73.082  32.510  1.00 10.72
ATOM   1701  CA  GLU A1008      69.028  73.410  31.892  1.00 10.72
ATOM   1702  C   GLU A1008      69.066  73.404  30.369  1.00 10.72
ATOM   1703  O   GLU A1008      70.144  73.771  29.757  1.00 10.72
ATOM   1704  CB  GLU A1008      70.098  72.429  32.417  1.00 39.30
ATOM   1705  CG  GLU A1008      69.942  70.977  31.916  1.00 39.30
ATOM   1706  CD  GLU A1008      69.159  70.091  32.896  1.00 39.30
ATOM   1707  OE1 GLU A1008      68.082  70.549  33.382  1.00 39.30
ATOM   1708  OE2 GLU A1008      69.634  68.944  33.178  1.00 39.30
ATOM   1710  N   SER A1009      67.976  72.880  29.764  1.00 31.45
ATOM   1711  CA  SER A1009      67.798  72.791  28.314  1.00 31.45
ATOM   1712  C   SER A1009      66.826  73.844  27.779  1.00 31.45
ATOM   1713  O   SER A1009      67.007  74.396  26.685  1.00 31.45
ATOM   1714  CB  SER A1009      67.286  71.410  27.930  1.00100.00
ATOM   1715  OG  SER A1009      68.088  70.402  28.500  1.00100.00
ATOM   1718  N   LEU A1010      65.745  74.095  28.485  1.00 75.06
ATOM   1719  CA  LEU A1010      64.852  75.103  27.977  1.00 75.06
ATOM   1720  C   LEU A1010      65.758  76.342  27.926  1.00 75.06
ATOM   1721  O   LEU A1010      65.737  77.146  26.989  1.00 75.06
ATOM   1722  CB  LEU A1010      63.675  75.238  28.938  1.00 62.28
ATOM   1723  CG  LEU A1010      62.685  74.078  28.725  1.00 62.28
ATOM   1724  CD1 LEU A1010      61.421  74.394  29.511  1.00 62.28
ATOM   1725  CD2 LEU A1010      62.379  73.854  27.229  1.00 62.28
ATOM   1727  N   ASN A1011      66.597  76.401  28.951  1.00 36.75
ATOM   1728  CA  ASN A1011      67.611  77.389  29.207  1.00 36.75
ATOM   1729  C   ASN A1011      68.761  77.280  28.189  1.00 36.75
ATOM   1730  O   ASN A1011      68.696  77.728  27.006  1.00 36.75
ATOM   1731  CB  ASN A1011      68.174  77.122  30.588  1.00 53.79
ATOM   1732  CG  ASN A1011      67.148  77.215  31.633  1.00 53.79
ATOM   1733  OD1 ASN A1011      66.008  77.430  31.335  1.00 53.79
ATOM   1734  ND2 ASN A1011      67.541  77.071  32.879  1.00 53.79
ATOM   1738  N   TYR A1012      69.810  76.638  28.685  1.00 25.53
ATOM   1739  CA  TYR A1012      71.016  76.422  27.940  1.00 25.53
ATOM   1740  C   TYR A1012      70.747  75.476  26.776  1.00 25.53
ATOM   1741  O   TYR A1012      71.392  75.570  25.756  1.00 25.53
ATOM   1742  CB  TYR A1012      72.118  75.898  28.872  1.00 38.16
ATOM   1743  CG  TYR A1012      71.934  76.312  30.315  1.00 38.16
ATOM   1744  CD1 TYR A1012      72.332  75.491  31.341  1.00 38.16
ATOM   1745  CD2 TYR A1012      71.301  77.512  30.645  1.00 38.16
ATOM   1746  CE1 TYR A1012      72.105  75.841  32.642  1.00 38.16
ATOM   1747  CE2 TYR A1012      71.072  77.863  31.943  1.00 38.16
ATOM   1748  CZ  TYR A1012      71.473  77.028  32.927  1.00 38.16
ATOM   1749  OH  TYR A1012      71.240  77.363  34.217  1.00 38.16
ATOM   1752  N   SER A1013      69.812  74.566  26.863  1.00 71.42
ATOM   1753  CA  SER A1013      69.638  73.752  25.672  1.00 71.42
ATOM   1754  C   SER A1013      70.875  72.864  25.398  1.00 71.42
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FIG. 6Y

ATOM	1755	O	SER	A1013	71.360	72.693	24.272	1.00	71.42
ATOM	1756	CB	SER	A1013	69.331	74.696	24.502	1.00	25.42
ATOM	1757	OG	SER	A1013	70.477	75.126	23.819	1.00	25.42
ATOM	1760	N	VAL	A1014	71.383	72.310	26.482	1.00	66.71
ATOM	1761	CA	VAL	A1014	72.507	71.433	26.395	1.00	66.71
ATOM	1762	C	VAL	A1014	71.902	70.215	26.967	1.00	66.71
ATOM	1763	O	VAL	A1014	71.255	70.283	27.994	1.00	66.71
ATOM	1764	CB	VAL	A1014	73.745	71.888	27.263	1.00	53.96
ATOM	1765	CG1	VAL	A1014	74.220	73.271	26.795	1.00	53.96
ATOM	1766	CG2	VAL	A1014	73.427	71.814	28.765	1.00	53.96
ATOM	1768	N	TYR	A1015	72.067	69.104	26.273	1.00	65.68
ATOM	1769	CA	TYR	A1015	71.511	67.861	26.751	1.00	65.68
ATOM	1770	C	TYR	A1015	72.584	66.891	27.248	1.00	65.68
ATOM	1771	O	TYR	A1015	73.635	66.702	26.646	1.00	65.68
ATOM	1772	CB	TYR	A1015	70.656	67.214	25.663	1.00	100.00
ATOM	1773	CG	TYR	A1015	69.758	68.179	24.939	1.00	100.00
ATOM	1774	CD1	TYR	A1015	70.148	68.741	23.734	1.00	100.00
ATOM	1775	CD2	TYR	A1015	68.509	68.505	25.434	1.00	100.00
ATOM	1776	CE1	TYR	A1015	69.315	69.596	23.037	1.00	100.00
ATOM	1777	CE2	TYR	A1015	67.664	69.364	24.740	1.00	100.00
ATOM	1778	CZ	TYR	A1015	68.078	69.901	23.546	1.00	100.00
ATOM	1779	OH	TYR	A1015	67.272	70.751	22.848	1.00	100.00
ATOM	1782	N	THR	A1016	72.263	66.269	28.363	1.00	55.88
ATOM	1783	CA	THR	A1016	73.124	65.322	29.008	1.00	55.88
ATOM	1784	C	THR	A1016	72.360	64.056	29.380	1.00	55.88
ATOM	1785	O	THR	A1016	71.164	63.996	29.243	1.00	55.88
ATOM	1786	CB	THR	A1016	73.653	65.988	30.209	1.00	30.90
ATOM	1787	OG1	THR	A1016	72.699	65.891	31.280	1.00	30.90
ATOM	1788	CG2	THR	A1016	73.881	67.440	29.876	1.00	30.90
ATOM	1791	N	THR	A1017	73.054	63.037	29.840	1.00	99.25
ATOM	1792	CA	THR	A1017	72.361	61.822	30.213	1.00	99.25
ATOM	1793	C	THR	A1017	71.878	62.074	31.618	1.00	99.25
ATOM	1794	O	THR	A1017	72.112	61.294	32.534	1.00	99.25
ATOM	1795	CB	THR	A1017	73.312	60.593	30.094	1.00	32.66
ATOM	1796	OG1	THR	A1017	72.893	59.789	28.972	1.00	32.66
ATOM	1797	CG2	THR	A1017	73.353	59.770	31.323	1.00	32.66
ATOM	1800	N	ASN	A1018	71.185	63.198	31.786	1.00	18.01
ATOM	1801	CA	ASN	A1018	70.687	63.569	33.141	1.00	18.01
ATOM	1802	C	ASN	A1018	69.349	64.119	32.874	1.00	18.01
ATOM	1803	O	ASN	A1018	68.447	64.021	33.724	1.00	18.01
ATOM	1804	CB	ASN	A1018	71.527	64.623	33.742	1.00	34.98
ATOM	1805	CG	ASN	A1018	71.808	64.337	35.101	1.00	34.98
ATOM	1806	OD1	ASN	A1018	71.282	64.966	35.982	1.00	34.98
ATOM	1807	ND2	ASN	A1018	72.659	63.353	35.331	1.00	34.98
ATOM	1811	N	SER	A1019	69.294	64.679	31.656	1.00	37.97
ATOM	1812	CA	SER	A1019	68.205	65.335	30.991	1.00	37.97
ATOM	1813	C	SER	A1019	67.811	64.369	29.862	1.00	37.97
ATOM	1814	O	SER	A1019	67.493	64.733	28.729	1.00	37.97
ATOM	1815	CB	SER	A1019	68.737	66.641	30.420	1.00	17.17
ATOM	1816	OG	SER	A1019	69.329	66.474	29.138	1.00	17.17
ATOM	1819	N	ASP	A1020	67.985	63.097	30.155	1.00	31.25
ATOM	1820	CA	ASP	A1020	67.582	62.062	29.225	1.00	31.25
ATOM	1821	C	ASP	A1020	66.669	61.475	30.328	1.00	31.25
ATOM	1822	O	ASP	A1020	65.473	61.257	30.127	1.00	31.25
ATOM	1823	CB	ASP	A1020	68.777	61.166	28.790	1.00	31.83
ATOM	1824	CG	ASP	A1020	69.074	61.295	27.302	1.00	31.83
ATOM	1825	OD1	ASP	A1020	68.289	61.870	26.618	1.00	31.83

FIG. 6Z

ATOM	1826	OD2	ASP	A1020	70.043	60.869	26.709	1.00	31.83
ATOM	1828	N	VAL	A1021	67.214	61.357	31.535	1.00	57.04
ATOM	1829	CA	VAL	A1021	66.440	60.813	32.614	1.00	57.04
ATOM	1830	C	VAL	A1021	65.131	61.522	32.628	1.00	57.04
ATOM	1831	O	VAL	A1021	64.091	60.915	32.317	1.00	57.04
ATOM	1832	CB	VAL	A1021	67.130	60.987	33.916	1.00	94.63
ATOM	1833	CG1	VAL	A1021	66.156	60.813	35.032	1.00	94.63
ATOM	1834	CG2	VAL	A1021	68.236	59.965	34.012	1.00	94.63
ATOM	1836	N	TRP	A1022	65.189	62.814	32.960	1.00	51.41
ATOM	1837	CA	TRP	A1022	64.023	63.696	33.032	1.00	51.41
ATOM	1838	C	TRP	A1022	63.002	63.457	31.908	1.00	51.41
ATOM	1839	O	TRP	A1022	61.815	63.252	32.147	1.00	51.41
ATOM	1840	CB	TRP	A1022	64.519	65.133	33.005	1.00	32.10
ATOM	1841	CG	TRP	A1022	63.422	66.227	32.925	1.00	32.10
ATOM	1842	CD1	TRP	A1022	62.602	66.469	31.868	1.00	32.10
ATOM	1843	CD2	TRP	A1022	63.068	67.160	33.938	1.00	32.10
ATOM	1844	NE1	TRP	A1022	61.779	67.469	32.157	1.00	32.10
ATOM	1845	CE2	TRP	A1022	62.032	67.931	33.428	1.00	32.10
ATOM	1846	CE3	TRP	A1022	63.526	67.420	35.221	1.00	32.10
ATOM	1847	CZ2	TRP	A1022	61.408	69.004	34.187	1.00	32.10
ATOM	1848	CZ3	TRP	A1022	62.921	68.481	35.978	1.00	32.10
ATOM	1849	CH2	TRP	A1022	61.879	69.255	35.453	1.00	32.10
ATOM	1852	N	SER	A1023	63.472	63.525	30.671	1.00	66.03
ATOM	1853	CA	SER	A1023	62.598	63.263	29.546	1.00	66.03
ATOM	1854	C	SER	A1023	61.921	61.955	29.911	1.00	66.03
ATOM	1855	O	SER	A1023	60.717	61.903	30.036	1.00	66.03
ATOM	1856	CB	SER	A1023	63.414	63.109	28.274	1.00	96.89
ATOM	1857	OG	SER	A1023	63.734	64.377	27.752	1.00	96.89
ATOM	1860	N	TYR	A1024	62.719	60.909	30.106	1.00	11.41
ATOM	1861	CA	TYR	A1024	62.238	59.645	30.472	1.00	11.41
ATOM	1862	C	TYR	A1024	60.940	59.597	31.308	1.00	11.41
ATOM	1863	O	TYR	A1024	60.018	58.807	30.992	1.00	11.41
ATOM	1864	CB	TYR	A1024	63.320	58.871	31.188	1.00	14.38
ATOM	1865	CG	TYR	A1024	62.850	57.491	31.472	1.00	14.38
ATOM	1866	CD1	TYR	A1024	62.821	56.581	30.474	1.00	14.38
ATOM	1867	CD2	TYR	A1024	62.314	57.167	32.733	1.00	14.38
ATOM	1868	CE1	TYR	A1024	62.276	55.380	30.688	1.00	14.38
ATOM	1869	CE2	TYR	A1024	61.765	55.987	32.993	1.00	14.38
ATOM	1870	CZ	TYR	A1024	61.734	55.069	31.972	1.00	14.38
ATOM	1871	OH	TYR	A1024	61.197	53.831	32.179	1.00	14.38
ATOM	1874	N	GLY	A1025	60.894	60.341	32.397	1.00	29.83
ATOM	1875	CA	GLY	A1025	59.678	60.385	33.207	1.00	29.83
ATOM	1876	C	GLY	A1025	58.509	61.033	32.430	1.00	29.83
ATOM	1877	O	GLY	A1025	57.356	60.716	32.652	1.00	29.83
ATOM	1879	N	VAL	A1026	58.762	61.985	31.554	1.00	67.56
ATOM	1880	CA	VAL	A1026	57.615	62.466	30.859	1.00	67.56
ATOM	1881	C	VAL	A1026	57.199	61.121	30.271	1.00	67.56
ATOM	1882	O	VAL	A1026	56.204	60.589	30.705	1.00	67.56
ATOM	1883	CB	VAL	A1026	57.975	63.548	29.836	1.00	59.88
ATOM	1884	CG1	VAL	A1026	56.872	64.579	29.759	1.00	59.88
ATOM	1885	CG2	VAL	A1026	59.232	64.199	30.249	1.00	59.88
ATOM	1887	N	LEU	A1027	57.982	60.546	29.354	1.00	31.95
ATOM	1888	CA	LEU	A1027	57.703	59.178	28.787	1.00	31.95
ATOM	1889	C	LEU	A1027	57.056	58.236	29.865	1.00	31.95
ATOM	1890	O	LEU	A1027	55.988	57.621	29.691	1.00	31.95
ATOM	1891	CB	LEU	A1027	59.000	58.502	28.304	1.00	37.14
ATOM	1892	CG	LEU	A1027	58.894	57.447	27.219	1.00	37.14

FIG. 6AA

ATOM	1893	CD1	LEU	A1027	57.496	57.117	27.007	1.00	37.14
ATOM	1894	CD2	LEU	A1027	59.417	57.890	25.930	1.00	37.14
ATOM	1896	N	LEU	A1028	57.746	58.125	30.978	1.00	8.77
ATOM	1897	CA	LEU	A1028	57.188	57.363	32.009	1.00	8.77
ATOM	1898	C	LEU	A1028	55.743	57.749	32.088	1.00	8.77
ATOM	1899	O	LEU	A1028	54.947	56.870	31.744	1.00	8.77
ATOM	1900	CB	LEU	A1028	57.875	57.508	33.363	1.00	48.45
ATOM	1901	CG	LEU	A1028	57.252	56.440	34.294	1.00	48.45
ATOM	1902	CD1	LEU	A1028	56.823	55.185	33.534	1.00	48.45
ATOM	1903	CD2	LEU	A1028	58.220	56.043	35.333	1.00	48.45
ATOM	1905	N	TRP	A1029	55.442	59.029	32.483	1.00	30.07
ATOM	1906	CA	TRP	A1029	54.084	59.703	32.660	1.00	30.07
ATOM	1907	C	TRP	A1029	53.253	59.613	31.429	1.00	30.07
ATOM	1908	O	TRP	A1029	52.118	59.261	31.397	1.00	30.07
ATOM	1909	CB	TRP	A1029	54.227	61.222	32.983	1.00	2.92
ATOM	1910	CG	TRP	A1029	52.932	62.000	33.312	1.00	2.92
ATOM	1911	CD1	TRP	A1029	52.349	62.276	34.582	1.00	2.92
ATOM	1912	CD2	TRP	A1029	51.964	62.434	32.334	1.00	2.92
ATOM	1913	NE1	TRP	A1029	51.050	62.846	34.369	1.00	2.92
ATOM	1914	CE2	TRP	A1029	50.827	62.919	33.011	1.00	2.92
ATOM	1915	CE3	TRP	A1029	51.955	62.444	30.937	1.00	2.92
ATOM	1916	CZ2	TRP	A1029	49.767	63.362	32.342	1.00	2.92
ATOM	1917	CZ3	TRP	A1029	50.836	62.910	30.283	1.00	2.92
ATOM	1918	CH2	TRP	A1029	49.791	63.345	30.971	1.00	2.92
ATOM	1921	N	GLU	A1030	53.881	60.008	30.382	1.00	26.20
ATOM	1922	CA	GLU	A1030	53.292	59.957	29.076	1.00	26.20
ATOM	1923	C	GLU	A1030	52.824	58.589	28.725	1.00	26.20
ATOM	1924	O	GLU	A1030	52.344	58.417	27.638	1.00	26.20
ATOM	1925	CB	GLU	A1030	54.358	60.378	28.077	1.00	24.00
ATOM	1926	CG	GLU	A1030	53.879	60.996	26.869	1.00	24.00
ATOM	1927	CD	GLU	A1030	54.860	60.718	25.857	1.00	24.00
ATOM	1928	OE1	GLU	A1030	55.885	60.279	26.378	1.00	24.00
ATOM	1929	OE2	GLU	A1030	54.661	60.907	24.633	1.00	24.00
ATOM	1931	N	ILE	A1031	52.969	57.631	29.631	1.00	14.69
ATOM	1932	CA	ILE	A1031	52.633	56.216	29.376	1.00	14.69
ATOM	1933	C	ILE	A1031	51.704	55.738	30.426	1.00	14.69
ATOM	1934	O	ILE	A1031	51.033	54.761	30.203	1.00	14.69
ATOM	1935	CB	ILE	A1031	53.923	55.272	29.416	1.00	33.44
ATOM	1936	CG1	ILE	A1031	54.294	54.757	28.021	1.00	33.44
ATOM	1937	CG2	ILE	A1031	53.671	53.993	30.253	1.00	33.44
ATOM	1938	CD1	ILE	A1031	55.762	54.225	27.948	1.00	33.44
ATOM	1940	N	VAL	A1032	51.726	56.285	31.621	1.00	14.19
ATOM	1941	CA	VAL	A1032	50.676	55.868	32.559	1.00	14.19
ATOM	1942	C	VAL	A1032	49.327	56.496	32.011	1.00	14.19
ATOM	1943	O	VAL	A1032	48.282	55.823	31.882	1.00	14.19
ATOM	1944	CB	VAL	A1032	50.924	56.349	33.944	1.00	41.51
ATOM	1945	CG1	VAL	A1032	49.666	56.640	34.596	1.00	41.51
ATOM	1946	CG2	VAL	A1032	51.681	55.290	34.704	1.00	41.51
ATOM	1948	N	SER	A1033	49.395	57.755	31.625	1.00	31.81
ATOM	1949	CA	SER	A1033	48.320	58.505	31.065	1.00	31.81
ATOM	1950	C	SER	A1033	47.658	57.730	29.910	1.00	31.81
ATOM	1951	O	SER	A1033	46.551	58.079	29.445	1.00	31.81
ATOM	1952	CB	SER	A1033	48.895	59.828	30.546	1.00	68.54
ATOM	1953	OG	SER	A1033	49.757	59.623	29.445	1.00	68.54
ATOM	1956	N	LEU	A1034	48.316	56.686	29.442	1.00	2.00
ATOM	1957	CA	LEU	A1034	47.777	55.984	28.298	1.00	2.00
ATOM	1958	C	LEU	A1034	47.645	56.833	26.999	1.00	2.00

FIG. 6BB

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ATOM   1959  O   LEU A1034      46.584  56.955  26.409  1.00  2.00
ATOM   1960  CB  LEU A1034      46.422  55.343  28.654  1.00 31.43
ATOM   1961  CG  LEU A1034      46.478  53.883  29.207  1.00 31.43
ATOM   1962  CD1 LEU A1034      45.072  53.333  29.484  1.00 31.43
ATOM   1963  CD2 LEU A1034      47.244  52.988  28.207  1.00 31.43
ATOM   1965  N   GLY A1035      48.706  57.372  26.438  1.00  4.53
ATOM   1966  CA  GLY A1035      48.437  58.149  25.224  1.00  4.53
ATOM   1967  C   GLY A1035      48.241  59.685  25.565  1.00  4.53
ATOM   1968  O   GLY A1035      47.964  60.498  24.649  1.00  4.53
ATOM   1970  N   GLY A1036      48.509  60.071  26.820  1.00 18.31
ATOM   1971  CA  GLY A1036      48.281  61.470  27.160  1.00 18.31
ATOM   1972  C   GLY A1036      49.211  62.717  27.185  1.00 18.31
ATOM   1973  O   GLY A1036      49.988  62.881  28.181  1.00 18.31
ATOM   1975  N   THR A1037      49.027  63.591  26.164  1.00 48.85
ATOM   1976  CA  THR A1037      49.733  64.890  25.939  1.00 48.85
ATOM   1977  C   THR A1037      50.225  65.522  27.265  1.00 48.85
ATOM   1978  O   THR A1037      49.431  65.933  28.077  1.00 48.85
ATOM   1979  CB  THR A1037      48.780  65.886  25.216  1.00 25.15
ATOM   1980  OG1 THR A1037      48.988  65.904  23.772  1.00 25.15
ATOM   1981  CG2 THR A1037      48.993  67.215  25.789  1.00 25.15
ATOM   1984  N   PRO A1038      51.538  65.697  27.456  1.00 42.23
ATOM   1985  CA  PRO A1038      51.796  66.239  28.775  1.00 42.23
ATOM   1986  C   PRO A1038      51.496  67.691  28.996  1.00 42.23
ATOM   1987  O   PRO A1038      51.359  68.450  28.057  1.00 42.23
ATOM   1988  CB  PRO A1038      53.271  65.779  29.048  1.00 10.66
ATOM   1989  CG  PRO A1038      53.679  65.007  27.861  1.00 10.66
ATOM   1990  CD  PRO A1038      52.809  65.456  26.765  1.00 10.66
ATOM   1991  N   TYR A1039      51.381  68.090  30.253  1.00 39.67
ATOM   1992  CA  TYR A1039      51.037  69.509  30.576  1.00 39.67
ATOM   1993  C   TYR A1039      49.924  69.987  29.682  1.00 39.67
ATOM   1994  O   TYR A1039      50.172  70.931  28.955  1.00 39.67
ATOM   1995  CB  TYR A1039      52.256  70.457  30.375  1.00 15.36
ATOM   1996  CG  TYR A1039      53.503  69.958  31.103  1.00 15.36
ATOM   1997  CD1 TYR A1039      54.685  69.536  30.407  1.00 15.36
ATOM   1998  CD2 TYR A1039      53.518  69.952  32.481  1.00 15.36
ATOM   1999  CE1 TYR A1039      55.790  69.157  31.105  1.00 15.36
ATOM   2000  CE2 TYR A1039      54.636  69.571  33.153  1.00 15.36
ATOM   2001  CZ  TYR A1039      55.737  69.191  32.449  1.00 15.36
ATOM   2002  OH  TYR A1039      56.737  68.889  33.251  1.00 15.36
ATOM   2005  N   CYS A1040      48.756  69.319  29.692  1.00100.00
ATOM   2006  CA  CYS A1040      47.597  69.681  28.845  1.00100.00
ATOM   2007  C   CYS A1040      47.013  70.930  29.435  1.00100.00
ATOM   2008  O   CYS A1040      46.711  70.987  30.625  1.00100.00
ATOM   2009  CB  CYS A1040      46.507  68.566  28.832  1.00 63.76
ATOM   2010  SG  CYS A1040      45.039  68.722  27.619  1.00 63.76
ATOM   2012  N   GLY A1041      46.836  71.938  28.605  1.00 75.53
ATOM   2013  CA  GLY A1041      46.305  73.175  29.127  1.00 75.53
ATOM   2014  C   GLY A1041      47.419  74.160  29.448  1.00 75.53
ATOM   2015  O   GLY A1041      47.217  75.358  29.342  1.00 75.53
ATOM   2017  N   MET A1042      48.581  73.668  29.868  1.00 27.54
ATOM   2018  CA  MET A1042      49.666  74.553  30.126  1.00 27.54
ATOM   2019  C   MET A1042      50.119  75.065  28.731  1.00 27.54
ATOM   2020  O   MET A1042      50.034  74.344  27.742  1.00 27.54
ATOM   2021  CB  MET A1042      50.771  73.851  30.909  1.00 47.82
ATOM   2022  CG  MET A1042      51.032  74.460  32.298  1.00 47.82
ATOM   2023  SD  MET A1042      52.810  74.502  32.805  1.00 47.82
ATOM   2024  CE  MET A1042      52.729  74.790  34.564  1.00 47.82
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FIG. 6CC

ATOM	2026	N	THR	A1043	50.481	76.351	28.681	1.00	59.25
ATOM	2027	CA	THR	A1043	50.918	77.067	27.468	1.00	59.25
ATOM	2028	C	THR	A1043	52.434	76.937	27.397	1.00	59.25
ATOM	2029	O	THR	A1043	53.084	76.835	28.437	1.00	59.25
ATOM	2030	CB	THR	A1043	50.586	78.617	27.528	1.00	62.50
ATOM	2031	OG1	THR	A1043	51.070	79.181	28.773	1.00	62.50
ATOM	2032	CG2	THR	A1043	49.076	78.877	27.351	1.00	62.50
ATOM	2035	N	CYS	A1044	52.997	76.968	26.194	1.00	100.00
ATOM	2036	CA	CYS	A1044	54.435	76.799	26.060	1.00	100.00
ATOM	2037	C	CYS	A1044	55.282	77.679	26.975	1.00	100.00
ATOM	2038	O	CYS	A1044	56.478	77.467	27.100	1.00	100.00
ATOM	2039	CB	CYS	A1044	54.857	76.963	24.601	1.00	77.67
ATOM	2040	SG	CYS	A1044	54.890	75.383	23.687	1.00	77.67
ATOM	2042	N	ALA	A1045	54.673	78.663	27.623	1.00	100.00
ATOM	2043	CA	ALA	A1045	55.425	79.501	28.548	1.00	100.00
ATOM	2044	C	ALA	A1045	54.810	79.446	29.910	1.00	100.00
ATOM	2045	O	ALA	A1045	55.455	79.833	30.878	1.00	100.00
ATOM	2046	CB	ALA	A1045	55.461	80.899	28.107	1.00	35.04
ATOM	2048	N	GLU	A1046	53.550	79.023	30.018	1.00	27.64
ATOM	2049	CA	GLU	A1046	53.057	78.932	31.346	1.00	27.64
ATOM	2050	C	GLU	A1046	54.177	78.018	31.917	1.00	27.64
ATOM	2051	O	GLU	A1046	54.507	78.117	33.092	1.00	27.64
ATOM	2052	CB	GLU	A1046	51.665	78.264	31.365	1.00	79.70
ATOM	2053	CG	GLU	A1046	50.465	79.239	31.521	1.00	79.70
ATOM	2054	CD	GLU	A1046	49.180	78.818	30.745	1.00	79.70
ATOM	2055	OE1	GLU	A1046	48.058	79.216	31.128	1.00	79.70
ATOM	2056	OE2	GLU	A1046	49.264	78.096	29.748	1.00	79.70
ATOM	2058	N	LEU	A1047	54.800	77.199	31.050	1.00	83.80
ATOM	2059	CA	LEU	A1047	55.871	76.230	31.413	1.00	83.80
ATOM	2060	C	LEU	A1047	57.286	76.737	31.646	1.00	83.80
ATOM	2061	O	LEU	A1047	57.838	76.529	32.712	1.00	83.80
ATOM	2062	CB	LEU	A1047	55.968	75.119	30.368	1.00	39.62
ATOM	2063	CG	LEU	A1047	55.167	73.857	30.626	1.00	39.62
ATOM	2064	CD1	LEU	A1047	55.186	73.119	29.339	1.00	39.62
ATOM	2065	CD2	LEU	A1047	55.697	73.034	31.803	1.00	39.62
ATOM	2067	N	TYR	A1048	57.904	77.315	30.615	1.00	32.07
ATOM	2068	CA	TYR	A1048	59.235	77.894	30.746	1.00	32.07
ATOM	2069	C	TYR	A1048	59.043	78.647	32.109	1.00	32.07
ATOM	2070	O	TYR	A1048	59.704	78.383	33.115	1.00	32.07
ATOM	2071	CB	TYR	A1048	59.498	78.877	29.566	1.00	14.15
ATOM	2072	CG	TYR	A1048	60.160	78.333	28.256	1.00	14.15
ATOM	2073	CD1	TYR	A1048	59.401	77.982	27.165	1.00	14.15
ATOM	2074	CD2	TYR	A1048	61.563	78.249	28.095	1.00	14.15
ATOM	2075	CE1	TYR	A1048	59.969	77.565	25.934	1.00	14.15
ATOM	2076	CE2	TYR	A1048	62.137	77.841	26.871	1.00	14.15
ATOM	2077	CZ	TYR	A1048	61.359	77.502	25.784	1.00	14.15
ATOM	2078	OH	TYR	A1048	61.927	77.135	24.513	1.00	14.15
ATOM	2081	N	GLU	A1049	58.055	79.533	32.169	1.00	36.64
ATOM	2082	CA	GLU	A1049	57.811	80.267	33.390	1.00	36.64
ATOM	2083	C	GLU	A1049	57.770	79.384	34.578	1.00	36.64
ATOM	2084	O	GLU	A1049	58.757	79.290	35.320	1.00	36.64
ATOM	2085	CB	GLU	A1049	56.500	81.002	33.368	1.00	35.78
ATOM	2086	CG	GLU	A1049	56.151	81.544	34.760	1.00	35.78
ATOM	2087	CD	GLU	A1049	54.683	81.875	34.899	1.00	35.78
ATOM	2088	OE1	GLU	A1049	53.989	82.043	33.858	1.00	35.78
ATOM	2089	OE2	GLU	A1049	54.252	81.947	36.060	1.00	35.78
ATOM	2091	N	LYS	A1050	56.601	78.737	34.708	1.00	93.85

FIG. 6DD

ATOM	2092	CA	LYS	A1050	56.197	77.839	35.793	1.00	93.85
ATOM	2093	C	LYS	A1050	57.046	76.622	36.085	1.00	93.85
ATOM	2094	O	LYS	A1050	57.178	76.212	37.231	1.00	93.85
ATOM	2095	CB	LYS	A1050	54.752	77.418	35.584	1.00	86.89
ATOM	2097	N	LEU	A1051	57.599	76.008	35.063	1.00	40.78
ATOM	2098	CA	LEU	A1051	58.458	74.868	35.336	1.00	40.78
ATOM	2099	C	LEU	A1051	59.412	75.166	36.508	1.00	40.78
ATOM	2100	O	LEU	A1051	59.321	74.483	37.539	1.00	40.78
ATOM	2101	CB	LEU	A1051	59.201	74.391	34.072	1.00	66.80
ATOM	2102	CG	LEU	A1051	58.984	72.898	33.726	1.00	66.80
ATOM	2103	CD1	LEU	A1051	57.754	72.376	34.370	1.00	66.80
ATOM	2104	CD2	LEU	A1051	58.875	72.719	32.253	1.00	66.80
ATOM	2106	N	PRO	A1052	60.356	76.129	36.369	1.00	42.79
ATOM	2107	CA	PRO	A1052	61.299	76.504	37.431	1.00	42.79
ATOM	2108	C	PRO	A1052	60.655	76.803	38.741	1.00	42.79
ATOM	2109	O	PRO	A1052	61.311	76.783	39.783	1.00	42.79
ATOM	2110	CB	PRO	A1052	61.928	77.731	36.906	1.00	29.07
ATOM	2111	CG	PRO	A1052	61.952	77.549	35.473	1.00	29.07
ATOM	2112	CD	PRO	A1052	60.713	76.805	35.110	1.00	29.07
ATOM	2113	N	GLN	A1053	59.365	77.114	38.699	1.00	68.39
ATOM	2114	CA	GLN	A1053	58.662	77.426	39.921	1.00	68.39
ATOM	2115	C	GLN	A1053	58.823	76.206	40.781	1.00	68.39
ATOM	2116	O	GLN	A1053	58.934	76.303	41.999	1.00	68.39
ATOM	2117	CB	GLN	A1053	57.200	77.701	39.646	1.00	100.00
ATOM	2119	N	GLY	A1054	58.852	75.049	40.125	1.00	93.49
ATOM	2120	CA	GLY	A1054	59.012	73.776	40.808	1.00	93.49
ATOM	2121	C	GLY	A1054	57.849	72.863	40.494	1.00	93.49
ATOM	2122	O	GLY	A1054	57.727	71.794	41.065	1.00	93.49
ATOM	2124	N	TYR	A1055	57.000	73.311	39.577	1.00	23.98
ATOM	2125	CA	TYR	A1055	55.804	72.609	39.141	1.00	23.98
ATOM	2126	C	TYR	A1055	56.207	71.481	38.197	1.00	23.98
ATOM	2127	O	TYR	A1055	57.062	71.702	37.321	1.00	23.98
ATOM	2128	CB	TYR	A1055	54.869	73.579	38.415	1.00	76.79
ATOM	2129	CG	TYR	A1055	53.703	72.894	37.769	1.00	76.79
ATOM	2130	CD1	TYR	A1055	52.547	72.645	38.480	1.00	76.79
ATOM	2131	CD2	TYR	A1055	53.803	72.391	36.479	1.00	76.79
ATOM	2132	CE1	TYR	A1055	51.516	71.891	37.927	1.00	76.79
ATOM	2133	CE2	TYR	A1055	52.788	71.639	35.913	1.00	76.79
ATOM	2134	CZ	TYR	A1055	51.647	71.382	36.644	1.00	76.79
ATOM	2135	OH	TYR	A1055	50.677	70.559	36.119	1.00	76.79
ATOM	2138	N	ARG	A1056	55.598	70.299	38.398	1.00	28.98
ATOM	2139	CA	ARG	A1056	55.836	69.092	37.633	1.00	28.98
ATOM	2140	C	ARG	A1056	54.472	68.506	37.281	1.00	28.98
ATOM	2141	O	ARG	A1056	53.443	68.997	37.844	1.00	28.98
ATOM	2142	CB	ARG	A1056	56.540	68.057	38.504	1.00	43.74
ATOM	2143	CG	ARG	A1056	57.930	68.420	39.046	1.00	43.74
ATOM	2144	CD	ARG	A1056	58.890	68.928	37.990	1.00	43.74
ATOM	2145	NE	ARG	A1056	59.420	70.184	38.476	1.00	43.74
ATOM	2146	CZ	ARG	A1056	60.710	70.421	38.632	1.00	43.74
ATOM	2147	NH1	ARG	A1056	61.589	69.481	38.326	1.00	43.74
ATOM	2148	NH2	ARG	A1056	61.113	71.570	39.153	1.00	43.74
ATOM	2155	N	LEU	A1057	54.457	67.425	36.423	1.00	3.73
ATOM	2156	CA	LEU	A1057	53.199	66.719	36.037	1.00	3.73
ATOM	2157	C	LEU	A1057	52.455	66.273	37.247	1.00	3.73
ATOM	2158	O	LEU	A1057	53.013	65.940	38.293	1.00	3.73
ATOM	2159	CB	LEU	A1057	53.453	65.540	35.129	1.00	53.30
ATOM	2160	CG	LEU	A1057	53.594	65.965	33.659	1.00	53.30

FIG. 6EE

ATOM	2161	CD1	LEU	A1057	54.129	64.770	32.869	1.00	53.30
ATOM	2162	CD2	LEU	A1057	52.271	66.541	33.071	1.00	53.30
ATOM	2164	N	GLU	A1058	51.138	66.322	37.070	1.00	13.17
ATOM	2165	CA	GLU	A1058	50.076	65.947	38.013	1.00	13.17
ATOM	2166	C	GLU	A1058	50.122	64.399	38.274	1.00	13.17
ATOM	2167	O	GLU	A1058	50.140	63.602	37.310	1.00	13.17
ATOM	2168	CB	GLU	A1058	48.779	66.341	37.327	1.00	48.21
ATOM	2169	CG	GLU	A1058	48.686	65.807	35.864	1.00	48.21
ATOM	2170	CD	GLU	A1058	49.433	66.661	34.827	1.00	48.21
ATOM	2171	OE1	GLU	A1058	50.080	67.619	35.269	1.00	48.21
ATOM	2172	OE2	GLU	A1058	49.379	66.410	33.589	1.00	48.21
ATOM	2174	N	LYS	A1059	50.163	63.947	39.531	1.00	35.98
ATOM	2175	CA	LYS	A1059	50.196	62.496	39.689	1.00	35.98
ATOM	2176	C	LYS	A1059	49.010	62.039	38.876	1.00	35.98
ATOM	2177	O	LYS	A1059	47.980	62.696	38.847	1.00	35.98
ATOM	2178	CB	LYS	A1059	50.046	62.040	41.118	1.00	48.90
ATOM	2179	CG	LYS	A1059	50.101	60.540	41.194	1.00	48.90
ATOM	2180	CD	LYS	A1059	50.190	60.048	42.616	1.00	48.90
ATOM	2181	CE	LYS	A1059	48.873	59.367	43.057	1.00	48.90
ATOM	2182	NZ	LYS	A1059	48.940	57.857	43.104	1.00	48.90
ATOM	2187	N	PRO	A1060	49.129	60.936	38.161	1.00	50.25
ATOM	2188	CA	PRO	A1060	47.931	60.601	37.405	1.00	50.25
ATOM	2189	C	PRO	A1060	46.928	59.608	37.964	1.00	50.25
ATOM	2190	O	PRO	A1060	47.176	58.424	37.967	1.00	50.25
ATOM	2191	CB	PRO	A1060	48.504	60.174	36.084	1.00	21.32
ATOM	2192	CG	PRO	A1060	50.037	59.963	36.356	1.00	21.32
ATOM	2193	CD	PRO	A1060	50.246	60.058	37.817	1.00	21.32
ATOM	2194	N	LEU	A1061	45.772	60.120	38.395	1.00	35.93
ATOM	2195	CA	LEU	A1061	44.633	59.371	38.985	1.00	35.93
ATOM	2196	C	LEU	A1061	44.746	57.870	39.239	1.00	35.93
ATOM	2197	O	LEU	A1061	44.731	57.415	40.396	1.00	35.93
ATOM	2198	CB	LEU	A1061	43.368	59.617	38.155	1.00	74.38
ATOM	2199	CG	LEU	A1061	43.355	59.574	36.617	1.00	74.38
ATOM	2200	CD1	LEU	A1061	44.689	59.971	35.997	1.00	74.38
ATOM	2201	CD2	LEU	A1061	42.942	58.174	36.185	1.00	74.38
ATOM	2203	N	ASN	A1062	44.864	57.145	38.117	1.00	56.10
ATOM	2204	CA	ASN	A1062	44.988	55.689	37.947	1.00	56.10
ATOM	2205	C	ASN	A1062	46.399	55.281	38.291	1.00	56.10
ATOM	2206	O	ASN	A1062	46.855	54.240	37.822	1.00	56.10
ATOM	2207	CB	ASN	A1062	44.865	55.366	36.477	1.00	38.56
ATOM	2208	CG	ASN	A1062	46.002	56.035	35.686	1.00	38.56
ATOM	2209	OD1	ASN	A1062	46.683	56.890	36.256	1.00	38.56
ATOM	2210	ND2	ASN	A1062	46.216	55.673	34.397	1.00	38.56
ATOM	2214	N	CYS	A1063	47.109	56.092	39.065	1.00	99.97
ATOM	2215	CA	CYS	A1063	48.503	55.791	39.376	1.00	99.97
ATOM	2216	C	CYS	A1063	48.861	55.613	40.829	1.00	99.97
ATOM	2217	O	CYS	A1063	48.362	56.299	41.699	1.00	99.97
ATOM	2218	CB	CYS	A1063	49.398	56.891	38.827	1.00	81.22
ATOM	2219	SG	CYS	A1063	50.449	56.431	37.527	1.00	81.22
ATOM	2221	N	ASP	A1064	49.770	54.691	41.070	1.00	40.11
ATOM	2222	CA	ASP	A1064	50.260	54.424	42.405	1.00	40.11
ATOM	2223	C	ASP	A1064	51.472	55.243	42.813	1.00	40.11
ATOM	2224	O	ASP	A1064	52.454	55.285	42.109	1.00	40.11
ATOM	2225	CB	ASP	A1064	50.623	52.961	42.560	1.00	60.57
ATOM	2226	CG	ASP	A1064	50.760	52.580	43.992	1.00	60.57
ATOM	2227	OD1	ASP	A1064	50.671	53.492	44.844	1.00	60.57
ATOM	2228	OD2	ASP	A1064	50.941	51.391	44.292	1.00	60.57

FIG. 6FF

```
ATOM   2230  N   ASP A1065      51.409  55.855  43.980  1.00 46.39
ATOM   2231  CA  ASP A1065      52.499  56.662  44.508  1.00 46.39
ATOM   2232  C   ASP A1065      53.884  56.043  44.229  1.00 46.39
ATOM   2233  O   ASP A1065      54.869  56.717  44.124  1.00 46.39
ATOM   2234  CB  ASP A1065      52.299  56.875  46.021  1.00 75.00
ATOM   2235  CG  ASP A1065      51.156  57.855  46.357  1.00 75.00
ATOM   2236  OD1 ASP A1065      50.426  58.300  45.452  1.00 75.00
ATOM   2237  OD2 ASP A1065      50.988  58.179  47.550  1.00 75.00
ATOM   2239  N   GLU A1066      53.951  54.742  44.107  1.00 29.06
ATOM   2240  CA  GLU A1066      55.205  54.101  43.803  1.00 29.06
ATOM   2241  C   GLU A1066      55.543  54.513  42.403  1.00 29.06
ATOM   2242  O   GLU A1066      56.559  55.189  42.220  1.00 29.06
ATOM   2243  CB  GLU A1066      55.109  52.567  43.888  1.00 46.46
ATOM   2244  CG  GLU A1066      56.488  51.877  43.895  1.00 46.46
ATOM   2245  CD  GLU A1066      56.612  50.697  44.880  1.00 46.46
ATOM   2246  OE1 GLU A1066      55.711  50.554  45.759  1.00 46.46
ATOM   2247  OE2 GLU A1066      57.616  49.923  44.765  1.00 46.46
ATOM   2249  N   VAL A1067      54.727  54.154  41.416  1.00 32.03
ATOM   2250  CA  VAL A1067      55.023  54.533  40.036  1.00 32.03
ATOM   2251  C   VAL A1067      55.293  56.054  39.731  1.00 32.03
ATOM   2252  O   VAL A1067      56.029  56.405  38.812  1.00 32.03
ATOM   2253  CB  VAL A1067      53.885  54.021  39.107  1.00 15.97
ATOM   2254  CG1 VAL A1067      53.965  54.642  37.618  1.00 15.97
ATOM   2255  CG2 VAL A1067      53.929  52.448  39.087  1.00 15.97
ATOM   2257  N   TYR A1068      54.738  56.973  40.480  1.00 40.19
ATOM   2258  CA  TYR A1068      55.001  58.328  40.091  1.00 40.19
ATOM   2259  C   TYR A1068      56.057  58.982  40.941  1.00 40.19
ATOM   2260  O   TYR A1068      56.899  59.755  40.422  1.00 40.19
ATOM   2261  CB  TYR A1068      53.684  59.082  40.070  1.00  3.92
ATOM   2262  CG  TYR A1068      53.658  60.503  40.344  1.00  3.92
ATOM   2263  CD1 TYR A1068      53.484  61.369  39.326  1.00  3.92
ATOM   2264  CD2 TYR A1068      53.650  60.958  41.607  1.00  3.92
ATOM   2265  CE1 TYR A1068      53.296  62.732  39.530  1.00  3.92
ATOM   2266  CE2 TYR A1068      53.473  62.266  41.862  1.00  3.92
ATOM   2267  CZ  TYR A1068      53.311  63.163  40.812  1.00  3.92
ATOM   2268  OH  TYR A1068      53.384  64.523  41.015  1.00  3.92
ATOM   2271  N   ASP A1069      55.999  58.711  42.242  1.00 34.55
ATOM   2272  CA  ASP A1069      57.036  59.211  43.139  1.00 34.55
ATOM   2273  C   ASP A1069      58.139  58.257  42.721  1.00 34.55
ATOM   2274  O   ASP A1069      58.415  57.326  43.454  1.00 34.55
ATOM   2275  CB  ASP A1069      56.639  58.964  44.588  1.00 80.97
ATOM   2276  CG  ASP A1069      57.819  58.905  45.514  1.00 80.97
ATOM   2277  OD1 ASP A1069      58.968  59.094  45.061  1.00 80.97
ATOM   2278  OD2 ASP A1069      57.591  58.673  46.714  1.00 80.97
ATOM   2280  N   LEU A1070      58.667  58.506  41.503  1.00  4.63
ATOM   2281  CA  LEU A1070      59.682  57.806  40.729  1.00  4.63
ATOM   2282  C   LEU A1070      59.701  58.504  39.408  1.00  4.63
ATOM   2283  O   LEU A1070      60.763  58.899  38.932  1.00  4.63
ATOM   2284  CB  LEU A1070      59.389  56.337  40.348  1.00 35.45
ATOM   2285  CG  LEU A1070      60.432  56.018  39.208  1.00 35.45
ATOM   2286  CD1 LEU A1070      61.722  55.660  39.890  1.00 35.45
ATOM   2287  CD2 LEU A1070      60.081  54.914  38.223  1.00 35.45
ATOM   2289  N   MET A1071      58.577  58.594  38.714  1.00 33.43
ATOM   2290  CA  MET A1071      58.562  59.377  37.490  1.00 33.43
ATOM   2291  C   MET A1071      59.072  60.795  37.999  1.00 33.43
ATOM   2292  O   MET A1071      59.717  61.547  37.301  1.00 33.43
ATOM   2293  CB  MET A1071      57.328  59.425  36.716  1.00 46.26
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FIG. 6GG

ATOM	2294	CG	MET	A1071	56.293	60.425	37.126	1.00	46.26
ATOM	2295	SD	MET	A1071	54.669	59.634	37.210	1.00	46.26
ATOM	2296	CE	MET	A1071	54.450	58.978	35.595	1.00	46.26
ATOM	2298	N	ARG	A1072	58.729	61.126	39.238	1.00	27.25
ATOM	2299	CA	ARG	A1072	59.114	62.389	39.800	1.00	27.25
ATOM	2300	C	ARG	A1072	60.612	62.482	40.123	1.00	27.25
ATOM	2301	O	ARG	A1072	61.232	63.557	40.039	1.00	27.25
ATOM	2302	CB	ARG	A1072	58.293	62.660	41.064	1.00	100.00
ATOM	2303	CG	ARG	A1072	56.890	63.206	40.805	1.00	100.00
ATOM	2304	CD	ARG	A1072	56.900	64.723	40.605	1.00	100.00
ATOM	2305	NE	ARG	A1072	57.085	65.438	41.861	1.00	100.00
ATOM	2306	CZ	ARG	A1072	56.517	66.600	42.150	1.00	100.00
ATOM	2307	NH1	ARG	A1072	55.722	67.184	41.271	1.00	100.00
ATOM	2308	NH2	ARG	A1072	56.749	67.178	43.315	1.00	100.00
ATOM	2315	N	GLN	A1073	61.212	61.376	40.533	1.00	63.04
ATOM	2316	CA	GLN	A1073	62.625	61.439	40.836	1.00	63.04
ATOM	2317	C	GLN	A1073	63.329	61.922	39.571	1.00	63.04
ATOM	2318	O	GLN	A1073	64.270	62.702	39.623	1.00	63.04
ATOM	2319	CB	GLN	A1073	63.152	60.060	41.233	1.00	85.05
ATOM	2320	CG	GLN	A1073	62.417	59.384	42.387	1.00	85.05
ATOM	2321	CD	GLN	A1073	63.134	58.127	42.896	1.00	85.05
ATOM	2322	OE1	GLN	A1073	62.615	57.410	43.752	1.00	85.05
ATOM	2323	NE2	GLN	A1073	64.322	57.859	42.364	1.00	85.05
ATOM	2327	N	CYS	A1074	62.838	61.488	38.421	1.00	37.06
ATOM	2328	CA	CYS	A1074	63.456	61.841	37.163	1.00	37.06
ATOM	2329	C	CYS	A1074	63.305	63.280	36.845	1.00	37.06
ATOM	2330	O	CYS	A1074	63.613	63.703	35.747	1.00	37.06
ATOM	2331	CB	CYS	A1074	62.838	61.039	36.021	1.00	55.92
ATOM	2332	SG	CYS	A1074	62.574	59.373	36.414	1.00	55.92
ATOM	2334	N	TRP	A1075	62.780	64.030	37.793	1.00	54.40
ATOM	2335	CA	TRP	A1075	62.549	65.443	37.559	1.00	54.40
ATOM	2336	C	TRP	A1075	63.051	66.360	38.693	1.00	54.40
ATOM	2337	O	TRP	A1075	62.683	67.533	38.757	1.00	54.40
ATOM	2338	CB	TRP	A1075	61.055	65.719	37.347	1.00	13.83
ATOM	2339	CG	TRP	A1075	60.306	65.009	36.268	1.00	13.83
ATOM	2340	CD1	TRP	A1075	60.694	64.793	34.985	1.00	13.83
ATOM	2341	CD2	TRP	A1075	58.962	64.566	36.350	1.00	13.83
ATOM	2342	NE1	TRP	A1075	59.683	64.256	34.259	1.00	13.83
ATOM	2343	CE2	TRP	A1075	58.593	64.109	35.078	1.00	13.83
ATOM	2344	CE3	TRP	A1075	58.029	64.518	37.373	1.00	13.83
ATOM	2345	CZ2	TRP	A1075	57.303	63.604	34.801	1.00	13.83
ATOM	2346	CZ3	TRP	A1075	56.751	64.011	37.074	1.00	13.83
ATOM	2347	CH2	TRP	A1075	56.423	63.573	35.814	1.00	13.83
ATOM	2350	N	ARG	A1076	63.867	65.842	39.597	1.00	99.49
ATOM	2351	CA	ARG	A1076	64.354	66.722	40.635	1.00	99.49
ATOM	2352	C	ARG	A1076	64.967	67.872	39.838	1.00	99.49
ATOM	2353	O	ARG	A1076	65.185	67.747	38.637	1.00	99.49
ATOM	2354	CB	ARG	A1076	65.412	66.011	41.484	1.00	96.28
ATOM	2355	CG	ARG	A1076	64.948	64.665	42.026	1.00	96.28
ATOM	2356	CD	ARG	A1076	65.966	64.028	42.968	1.00	96.28
ATOM	2357	NE	ARG	A1076	65.361	63.411	44.155	1.00	96.28
ATOM	2358	CZ	ARG	A1076	65.408	62.110	44.427	1.00	96.28
ATOM	2359	NH1	ARG	A1076	66.029	61.286	43.595	1.00	96.28
ATOM	2360	NH2	ARG	A1076	64.855	61.635	45.538	1.00	96.28
ATOM	2367	N	GLU	A1077	65.200	69.008	40.469	1.00	54.46
ATOM	2368	CA	GLU	A1077	65.824	70.107	39.764	1.00	54.46
ATOM	2369	C	GLU	A1077	67.293	69.771	39.587	1.00	54.46

FIG. 6HH

ATOM	2370	O	GLU	A1077	67.727	69.428	38.509	1.00	54.46
ATOM	2371	CB	GLU	A1077	65.689	71.328	40.555	1.00	10.55
ATOM	2373	N	LYS	A1078	68.050	69.854	40.670	1.00	35.40
ATOM	2374	CA	LYS	A1078	69.476	69.542	40.642	1.00	35.40
ATOM	2375	C	LYS	A1078	69.746	68.345	39.704	1.00	35.40
ATOM	2376	O	LYS	A1078	69.592	67.215	40.099	1.00	35.40
ATOM	2377	CB	LYS	A1078	69.954	69.234	42.058	1.00	95.51
ATOM	2378	CG	LYS	A1078	70.054	70.458	42.936	1.00	95.51
ATOM	2379	CD	LYS	A1078	70.070	70.094	44.414	1.00	95.51
ATOM	2380	CE	LYS	A1078	71.487	70.050	44.990	1.00	95.51
ATOM	2381	NZ	LYS	A1078	71.575	69.341	46.309	1.00	95.51
ATOM	2386	N	PRO	A1079	70.230	68.582	38.481	1.00	54.45
ATOM	2387	CA	PRO	A1079	70.437	67.398	37.643	1.00	54.45
ATOM	2388	C	PRO	A1079	71.172	66.206	38.238	1.00	54.45
ATOM	2389	O	PRO	A1079	70.745	65.097	38.040	1.00	54.45
ATOM	2390	CB	PRO	A1079	71.099	67.958	36.381	1.00	46.70
ATOM	2391	CG	PRO	A1079	70.732	69.385	36.376	1.00	46.70
ATOM	2392	CD	PRO	A1079	70.658	69.817	37.801	1.00	46.70
ATOM	2393	N	TYR	A1080	72.265	66.402	38.968	1.00	100.00
ATOM	2394	CA	TYR	A1080	72.963	65.243	39.542	1.00	100.00
ATOM	2395	C	TYR	A1080	72.128	64.578	40.621	1.00	100.00
ATOM	2396	O	TYR	A1080	72.619	63.747	41.375	1.00	100.00
ATOM	2397	CB	TYR	A1080	74.301	65.630	40.141	1.00	41.54
ATOM	2398	CG	TYR	A1080	74.194	66.859	40.985	1.00	41.54
ATOM	2399	CD1	TYR	A1080	73.912	66.774	42.320	1.00	41.54
ATOM	2400	CD2	TYR	A1080	74.316	68.109	40.422	1.00	41.54
ATOM	2401	CE1	TYR	A1080	73.757	67.883	43.061	1.00	41.54
ATOM	2402	CE2	TYR	A1080	74.158	69.220	41.161	1.00	41.54
ATOM	2403	CZ	TYR	A1080	73.882	69.118	42.480	1.00	41.54
ATOM	2404	OH	TYR	A1080	73.778	70.273	43.233	1.00	41.54
ATOM	2407	N	GLU	A1081	70.870	64.982	40.712	1.00	38.29
ATOM	2408	CA	GLU	A1081	69.948	64.379	41.652	1.00	38.29
ATOM	2409	C	GLU	A1081	69.030	63.423	40.853	1.00	38.29
ATOM	2410	O	GLU	A1081	68.522	62.448	41.398	1.00	38.29
ATOM	2411	CB	GLU	A1081	69.214	65.451	42.451	1.00	37.33
ATOM	2412	CG	GLU	A1081	69.927	65.679	43.797	1.00	37.33
ATOM	2413	CD	GLU	A1081	69.529	66.957	44.542	1.00	37.33
ATOM	2414	OE1	GLU	A1081	70.080	67.203	45.646	1.00	37.33
ATOM	2415	OE2	GLU	A1081	68.676	67.741	44.045	1.00	37.33
ATOM	2417	N	ARG	A1082	68.876	63.690	39.550	1.00	35.27
ATOM	2418	CA	ARG	A1082	68.154	62.803	38.655	1.00	35.27
ATOM	2419	C	ARG	A1082	68.831	61.404	38.883	1.00	35.27
ATOM	2420	O	ARG	A1082	69.932	61.322	39.463	1.00	35.27
ATOM	2421	CB	ARG	A1082	68.336	63.260	37.216	1.00	62.49
ATOM	2422	CG	ARG	A1082	67.202	64.072	36.647	1.00	62.49
ATOM	2423	CD	ARG	A1082	67.299	65.548	36.942	1.00	62.49
ATOM	2424	NE	ARG	A1082	67.442	66.375	35.737	1.00	62.49
ATOM	2425	CZ	ARG	A1082	67.099	67.665	35.661	1.00	62.49
ATOM	2426	NH1	ARG	A1082	66.585	68.293	36.705	1.00	62.49
ATOM	2427	NH2	ARG	A1082	67.317	68.345	34.547	1.00	62.49
ATOM	2434	N	PRO	A1083	68.144	60.280	38.530	1.00	37.62
ATOM	2435	CA	PRO	A1083	68.732	58.945	38.729	1.00	37.62
ATOM	2436	C	PRO	A1083	69.270	58.328	37.461	1.00	37.62
ATOM	2437	O	PRO	A1083	68.905	58.780	36.414	1.00	37.62
ATOM	2438	CB	PRO	A1083	67.541	58.148	39.267	1.00	40.57
ATOM	2439	CG	PRO	A1083	66.294	59.139	39.213	1.00	40.57
ATOM	2440	CD	PRO	A1083	66.721	60.125	38.171	1.00	40.57

FIG. 6II

ATOM	2441	N	SER	A1084	70.157	57.337	37.541	1.00	23.77
ATOM	2442	CA	SER	A1084	70.642	56.597	36.339	1.00	23.77
ATOM	2443	C	SER	A1084	69.465	55.689	35.826	1.00	23.77
ATOM	2444	O	SER	A1084	68.690	55.172	36.633	1.00	23.77
ATOM	2445	CB	SER	A1084	71.772	55.617	36.733	1.00	2.00
ATOM	2446	OG	SER	A1084	71.518	55.019	38.069	1.00	2.00
ATOM	2449	N	PHE	A1085	69.330	55.466	34.520	1.00	44.36
ATOM	2450	CA	PHE	A1085	68.272	54.565	34.032	1.00	44.36
ATOM	2451	C	PHE	A1085	68.458	53.237	34.801	1.00	44.36
ATOM	2452	O	PHE	A1085	67.633	52.852	35.603	1.00	44.36
ATOM	2453	CB	PHE	A1085	68.414	54.399	32.529	1.00	95.75
ATOM	2454	CG	PHE	A1085	68.175	55.669	31.783	1.00	95.75
ATOM	2455	CD1	PHE	A1085	69.088	56.137	30.866	1.00	95.75
ATOM	2456	CD2	PHE	A1085	67.036	56.409	32.022	1.00	95.75
ATOM	2457	CE1	PHE	A1085	68.863	57.321	30.200	1.00	95.75
ATOM	2458	CE2	PHE	A1085	66.807	57.591	31.361	1.00	95.75
ATOM	2459	CZ	PHE	A1085	67.713	58.049	30.452	1.00	95.75
ATOM	2461	N	ALA	A1086	69.541	52.541	34.541	1.00	35.91
ATOM	2462	CA	ALA	A1086	69.894	51.395	35.347	1.00	35.91
ATOM	2463	C	ALA	A1086	69.171	51.316	36.743	1.00	35.91
ATOM	2464	O	ALA	A1086	68.741	50.223	37.179	1.00	35.91
ATOM	2465	CB	ALA	A1086	71.400	51.423	35.580	1.00	44.62
ATOM	2467	N	GLN	A1087	69.081	52.427	37.464	1.00	20.15
ATOM	2468	CA	GLN	A1087	68.394	52.412	38.732	1.00	20.15
ATOM	2469	C	GLN	A1087	66.842	52.338	38.466	1.00	20.15
ATOM	2470	O	GLN	A1087	66.039	51.538	39.059	1.00	20.15
ATOM	2471	CB	GLN	A1087	68.766	53.690	39.501	1.00	19.20
ATOM	2472	CG	GLN	A1087	70.227	53.686	40.069	1.00	19.20
ATOM	2473	CD	GLN	A1087	70.563	54.908	40.926	1.00	19.20
ATOM	2474	OE1	GLN	A1087	70.927	55.939	40.379	1.00	19.20
ATOM	2475	NE2	GLN	A1087	70.473	54.783	42.263	1.00	19.20
ATOM	2479	N	ILE	A1088	66.451	53.197	37.550	1.00	25.82
ATOM	2480	CA	ILE	A1088	65.088	53.310	37.160	1.00	25.82
ATOM	2481	C	ILE	A1088	64.852	51.851	36.847	1.00	25.82
ATOM	2482	O	ILE	A1088	63.966	51.300	37.447	1.00	25.82
ATOM	2483	CB	ILE	A1088	64.921	54.260	35.919	1.00	17.84
ATOM	2484	CG1	ILE	A1088	65.069	55.704	36.340	1.00	17.84
ATOM	2485	CG2	ILE	A1088	63.626	53.984	35.170	1.00	17.84
ATOM	2486	CD1	ILE	A1088	65.738	56.545	35.203	1.00	17.84
ATOM	2488	N	LEU	A1089	65.628	51.205	35.969	1.00	19.62
ATOM	2489	CA	LEU	A1089	65.380	49.747	35.692	1.00	19.62
ATOM	2490	C	LEU	A1089	65.471	48.746	36.793	1.00	19.62
ATOM	2491	O	LEU	A1089	64.899	47.746	36.680	1.00	19.62
ATOM	2492	CB	LEU	A1089	66.155	49.127	34.566	1.00	2.73
ATOM	2493	CG	LEU	A1089	65.363	47.882	33.978	1.00	2.73
ATOM	2494	CD1	LEU	A1089	65.305	47.787	32.425	1.00	2.73
ATOM	2495	CD2	LEU	A1089	66.127	46.642	34.338	1.00	2.73
ATOM	2497	N	VAL	A1090	66.164	48.988	37.866	1.00	15.82
ATOM	2498	CA	VAL	A1090	66.074	47.993	38.898	1.00	15.82
ATOM	2499	C	VAL	A1090	64.931	48.400	39.791	1.00	15.82
ATOM	2500	O	VAL	A1090	64.700	47.776	40.834	1.00	15.82
ATOM	2501	CB	VAL	A1090	67.396	47.811	39.695	1.00	8.61
ATOM	2502	CG1	VAL	A1090	67.259	48.053	41.220	1.00	8.61
ATOM	2503	CG2	VAL	A1090	67.829	46.397	39.452	1.00	8.61
ATOM	2505	N	SER	A1091	64.218	49.451	39.377	1.00	45.24
ATOM	2506	CA	SER	A1091	63.073	50.005	40.110	1.00	45.24
ATOM	2507	C	SER	A1091	61.708	49.486	39.628	1.00	45.24

FIG. 6JJ

```
ATOM   2508  O   SER A1091      60.764  49.305  40.422  1.00 45.24
ATOM   2509  CB  SER A1091      63.064  51.511  39.963  1.00 46.04
ATOM   2510  OG  SER A1091      62.473  52.119  41.083  1.00 46.04
ATOM   2513  N   LEU A1092      61.582  49.317  38.318  1.00 48.10
ATOM   2514  CA  LEU A1092      60.336  48.814  37.772  1.00 48.10
ATOM   2515  C   LEU A1092      60.362  47.286  37.896  1.00 48.10
ATOM   2516  O   LEU A1092      59.310  46.649  38.093  1.00 48.10
ATOM   2517  CB  LEU A1092      60.226  49.217  36.335  1.00 20.50
ATOM   2518  CG  LEU A1092      60.649  50.636  36.171  1.00 20.50
ATOM   2519  CD1 LEU A1092      61.112  50.957  34.819  1.00 20.50
ATOM   2520  CD2 LEU A1092      59.492  51.389  36.445  1.00 20.50
ATOM   2522  N   ASN A1093      61.588  46.721  37.764  1.00 21.90
ATOM   2523  CA  ASN A1093      61.816  45.284  37.914  1.00 21.90
ATOM   2524  C   ASN A1093      61.298  44.970  39.321  1.00 21.90
ATOM   2525  O   ASN A1093      60.506  44.064  39.515  1.00 21.90
ATOM   2526  CB  ASN A1093      63.301  45.010  37.802  1.00 40.34
ATOM   2527  CG  ASN A1093      63.756  44.903  36.364  1.00 40.34
ATOM   2528  OD1 ASN A1093      64.796  44.322  36.103  1.00 40.34
ATOM   2529  ND2 ASN A1093      62.989  45.468  35.422  1.00 40.34
ATOM   2533  N   ARG A1094      61.699  45.746  40.314  1.00 34.76
ATOM   2534  CA  ARG A1094      61.194  45.385  41.611  1.00 34.76
ATOM   2535  C   ARG A1094      59.685  45.221  41.451  1.00 34.76
ATOM   2536  O   ARG A1094      59.122  44.320  42.022  1.00 34.76
ATOM   2537  CB  ARG A1094      61.515  46.451  42.653  1.00 99.74
ATOM   2538  CG  ARG A1094      61.377  45.969  44.088  1.00 99.74
ATOM   2539  CD  ARG A1094      59.934  46.037  44.575  1.00 99.74
ATOM   2540  NE  ARG A1094      59.736  47.099  45.557  1.00 99.74
ATOM   2541  CZ  ARG A1094      58.550  47.590  45.907  1.00 99.74
ATOM   2542  NH1 ARG A1094      57.438  47.117  45.357  1.00 99.74
ATOM   2543  NH2 ARG A1094      58.479  48.565  46.805  1.00 99.74
ATOM   2550  N   MET A1095      59.045  46.073  40.640  1.00 52.46
ATOM   2551  CA  MET A1095      57.594  46.029  40.452  1.00 52.46
ATOM   2552  C   MET A1095      57.136  44.721  39.781  1.00 52.46
ATOM   2553  O   MET A1095      56.663  43.809  40.435  1.00 52.46
ATOM   2554  CB  MET A1095      57.151  47.287  39.683  1.00 62.45
ATOM   2555  CG  MET A1095      57.076  48.578  40.594  1.00 62.45
ATOM   2556  SD  MET A1095      57.031  50.297  39.847  1.00 62.45
ATOM   2557  CE  MET A1095      57.509  51.299  41.162  1.00 62.45
ATOM   2559  N   LEU A1096      57.289  44.666  38.476  1.00 14.04
ATOM   2560  CA  LEU A1096      57.029  43.531  37.600  1.00 14.04
ATOM   2561  C   LEU A1096      57.039  42.101  38.255  1.00 14.04
ATOM   2562  O   LEU A1096      56.575  41.148  37.638  1.00 14.04
ATOM   2563  CB  LEU A1096      58.046  43.560  36.441  1.00 37.25
ATOM   2564  CG  LEU A1096      58.047  44.610  35.300  1.00 37.25
ATOM   2565  CD1 LEU A1096      59.158  44.291  34.269  1.00 37.25
ATOM   2566  CD2 LEU A1096      56.643  44.684  34.592  1.00 37.25
ATOM   2568  N   GLU A1097      57.574  41.928  39.450  1.00 42.58
ATOM   2569  CA  GLU A1097      57.530  40.621  40.048  1.00 42.58
ATOM   2570  C   GLU A1097      56.651  40.690  41.296  1.00 42.58
ATOM   2571  O   GLU A1097      57.019  40.286  42.411  1.00 42.58
ATOM   2572  CB  GLU A1097      58.919  40.136  40.396  1.00100.00
ATOM   2573  CG  GLU A1097      59.757  39.901  39.188  1.00100.00
ATOM   2574  CD  GLU A1097      60.925  40.839  39.144  1.00100.00
ATOM   2575  OE1 GLU A1097      61.083  41.611  40.117  1.00100.00
ATOM   2576  OE2 GLU A1097      61.680  40.799  38.147  1.00100.00
ATOM   2578  N   GLU A1098      55.454  41.211  41.108  1.00 43.50
ATOM   2579  CA  GLU A1098      54.540  41.313  42.226  1.00 43.50
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FIG. 6KK

ATOM	2580	C	GLU	A1098	53.112	41.239	41.679	1.00	43.50
ATOM	2581	O	GLU	A1098	52.247	40.533	42.228	1.00	43.50
ATOM	2582	CB	GLU	A1098	54.783	42.639	42.970	1.00	60.12
ATOM	2583	CG	GLU	A1098	56.233	43.014	43.093	1.00	60.12
ATOM	2584	CD	GLU	A1098	56.895	42.498	44.392	1.00	60.12
ATOM	2585	OE1	GLU	A1098	56.253	42.586	45.481	1.00	60.12
ATOM	2586	OE2	GLU	A1098	58.071	42.019	44.331	1.00	60.12
ATOM	2588	N	ARG	A1099	52.896	41.931	40.566	1.00	100.00
ATOM	2589	CA	ARG	A1099	51.564	42.010	40.005	1.00	100.00
ATOM	2590	C	ARG	A1099	50.792	42.471	41.232	1.00	100.00
ATOM	2591	O	ARG	A1099	50.117	41.681	41.899	1.00	100.00
ATOM	2592	CB	ARG	A1099	51.050	40.643	39.530	1.00	69.49
ATOM	2593	CG	ARG	A1099	49.707	40.745	38.761	1.00	69.49
ATOM	2594	CD	ARG	A1099	49.883	40.941	37.244	1.00	69.49
ATOM	2595	NE	ARG	A1099	49.647	42.326	36.812	1.00	69.49
ATOM	2596	CZ	ARG	A1099	49.095	42.672	35.648	1.00	69.49
ATOM	2597	NH1	ARG	A1099	48.705	41.740	34.782	1.00	69.49
ATOM	2598	NH2	ARG	A1099	48.989	43.951	35.322	1.00	69.49
ATOM	2605	N	LYS	A1100	50.957	43.748	41.555	1.00	49.25
ATOM	2606	CA	LYS	A1100	50.308	44.328	42.698	1.00	49.25
ATOM	2607	C	LYS	A1100	49.232	45.070	42.019	1.00	49.25
ATOM	2608	O	LYS	A1100	48.111	45.129	42.502	1.00	49.25
ATOM	2609	CB	LYS	A1100	51.247	45.296	43.419	1.00	99.82
ATOM	2610	CG	LYS	A1100	50.853	45.635	44.859	1.00	99.82
ATOM	2611	CD	LYS	A1100	50.997	44.447	45.815	1.00	99.82
ATOM	2612	CE	LYS	A1100	49.635	43.868	46.212	1.00	99.82
ATOM	2613	NZ	LYS	A1100	49.247	44.148	47.622	1.00	99.82
ATOM	2618	N	THR	A1101	49.603	45.578	40.850	1.00	64.74
ATOM	2619	CA	THR	A1101	48.769	46.370	39.946	1.00	64.74
ATOM	2620	C	THR	A1101	49.030	47.835	40.194	1.00	64.74
ATOM	2621	O	THR	A1101	48.381	48.463	41.014	1.00	64.74
ATOM	2622	CB	THR	A1101	47.282	46.080	40.069	1.00	100.00
ATOM	2623	OG1	THR	A1101	47.083	44.676	40.244	1.00	100.00
ATOM	2624	CG2	THR	A1101	46.581	46.494	38.801	1.00	100.00
ATOM	2627	N	TYR	A1102	50.026	48.346	39.472	1.00	78.61
ATOM	2628	CA	TYR	A1102	50.462	49.715	39.571	1.00	78.61
ATOM	2629	C	TYR	A1102	49.666	50.619	38.672	1.00	78.61
ATOM	2630	O	TYR	A1102	49.438	51.753	39.026	1.00	78.61
ATOM	2631	CB	TYR	A1102	51.960	49.856	39.210	1.00	42.69
ATOM	2632	CG	TYR	A1102	52.910	49.107	40.092	1.00	42.69
ATOM	2633	CD1	TYR	A1102	53.228	47.735	39.812	1.00	42.69
ATOM	2634	CD2	TYR	A1102	53.356	49.663	41.288	1.00	42.69
ATOM	2635	CE1	TYR	A1102	53.926	46.943	40.711	1.00	42.69
ATOM	2636	CE2	TYR	A1102	54.061	48.880	42.207	1.00	42.69
ATOM	2637	CZ	TYR	A1102	54.327	47.512	41.917	1.00	42.69
ATOM	2638	OH	TYR	A1102	54.871	46.698	42.873	1.00	42.69
ATOM	2641	N	VAL	A1103	49.233	50.151	37.513	1.00	100.00
ATOM	2642	CA	VAL	A1103	48.509	51.066	36.650	1.00	100.00
ATOM	2643	C	VAL	A1103	47.068	50.762	36.293	1.00	100.00
ATOM	2644	O	VAL	A1103	46.757	50.368	35.175	1.00	100.00
ATOM	2645	CB	VAL	A1103	49.276	51.326	35.350	1.00	100.00
ATOM	2646	CG1	VAL	A1103	48.590	52.426	34.565	1.00	100.00
ATOM	2647	CG2	VAL	A1103	50.694	51.746	35.661	1.00	100.00
ATOM	2649	N	ASN	A1104	46.191	50.990	37.260	1.00	30.52
ATOM	2650	CA	ASN	A1104	44.768	50.802	37.118	1.00	30.52
ATOM	2651	C	ASN	A1104	44.245	51.216	35.761	1.00	30.52
ATOM	2652	O	ASN	A1104	44.475	52.317	35.289	1.00	30.52

FIG. 6LL

```
ATOM   2653  CB  ASN A1104      44.041  51.572  38.171  1.00 63.62
ATOM   2654  CG  ASN A1104      42.646  51.154  38.272  1.00 63.62
ATOM   2655  OD1 ASN A1104      41.934  51.137  37.275  1.00 63.62
ATOM   2656  ND2 ASN A1104      42.224  50.788  39.469  1.00 63.62
ATOM   2660  N   THR A1105      43.519  50.305  35.135  1.00 45.33
ATOM   2661  CA  THR A1105      42.978  50.501  33.817  1.00 45.33
ATOM   2662  C   THR A1105      41.629  49.786  33.751  1.00 45.33
ATOM   2663  O   THR A1105      40.980  49.726  32.734  1.00 45.33
ATOM   2664  CB  THR A1105      43.987  49.959  32.817  1.00 46.03
ATOM   2665  OG1 THR A1105      44.604  48.759  33.328  1.00 46.03
ATOM   2666  CG2 THR A1105      45.083  50.972  32.633  1.00 46.03
ATOM   2669  N   THR A1105      41.199  49.243  34.869  1.00 15.59
ATOM   2670  CA  THR A1106      39.900  48.589  34.956  1.00 15.59
ATOM   2671  C   THR A1106      38.820  49.661  35.289  1.00 15.59
ATOM   2672  O   THR A1106      39.072  50.461  36.167  1.00 15.59
ATOM   2673  CB  THR A1106      39.931  47.514  36.091  1.00 59.09
ATOM   2674  OG1 THR A1106      39.776  46.205  35.525  1.00 59.09
ATOM   2675  CG2 THR A1106      38.827  47.743  37.083  1.00 59.09
ATOM   2678  N   LEU A1107      37.641  49.683  34.662  1.00 27.67
ATOM   2679  CA  LEU A1107      36.613  50.729  35.028  1.00 27.67
ATOM   2680  C   LEU A1107      35.966  50.401  36.392  1.00 27.67
ATOM   2681  O   LEU A1107      34.939  49.735  36.477  1.00 27.67
ATOM   2682  CB  LEU A1107      35.491  50.874  33.967  1.00 39.85
ATOM   2683  CG  LEU A1107      35.834  50.768  32.492  1.00 39.85
ATOM   2684  CD1 LEU A1107      34.611  50.486  31.731  1.00 39.85
ATOM   2685  CD2 LEU A1107      36.500  51.981  31.985  1.00 39.85
ATOM   2687  N   TYR A1108      36.576  50.816  37.480  1.00 99.39
ATOM   2688  CA  TYR A1108      35.969  50.482  38.748  1.00 99.39
ATOM   2689  C   TYR A1108      34.685  51.305  38.878  1.00 99.39
ATOM   2690  O   TYR A1108      33.900  51.097  39.806  1.00 99.39
ATOM   2691  CB  TYR A1108      36.973  50.749  39.872  1.00100.00
ATOM   2692  CG  TYR A1108      38.383  50.249  39.513  1.00100.00
ATOM   2693  CD1 TYR A1108      39.286  51.419  39.214  1.00100.00
ATOM   2694  CD2 TYR A1108      38.945  49.421  40.644  1.00100.00
ATOM   2696  N   GLU A1109      34.486  52.198  37.899  1.00100.00
ATOM   2697  CA  GLU A1109      33.341  53.116  37.779  1.00100.00
ATOM   2698  C   GLU A1109      33.875  54.536  37.598  1.00100.00
ATOM   2699  O   GLU A1109      34.957  54.846  38.095  1.00100.00
ATOM   2700  CB  GLU A1109      32.454  53.065  39.001  1.00 76.82
ATOM   2702  N   LYS A1110      33.104  55.390  36.914  1.00100.00
ATOM   2703  CA  LYS A1110      33.486  56.779  36.626  1.00100.00
ATOM   2704  C   LYS A1110      34.891  56.830  36.038  1.00100.00
ATOM   2705  O   LYS A1110      35.858  56.673  36.763  1.00100.00
ATOM   2706  CB  LYS A1110      33.430  57.631  37.900  1.00 99.15
ATOM   2707  CG  LYS A1110      34.009  56.977  39.152  1.00 99.15
ATOM   2708  CD  LYS A1110      34.718  57.970  40.052  1.00 99.15
ATOM   2709  CE  LYS A1110      34.246  57.852  41.490  1.00 99.15
ATOM   2710  NZ  LYS A1110      33.479  59.054  41.919  1.00 99.15
ATOM   2715  N   PHE A1111      35.030  57.055  34.737  1.00100.00
ATOM   2716  CA  PHE A1111      36.373  57.068  34.186  1.00100.00
ATOM   2717  C   PHE A1111      36.824  58.244  33.333  1.00100.00
ATOM   2718  O   PHE A1111      36.116  58.763  32.487  1.00100.00
ATOM   2719  CB  PHE A1111      36.685  55.747  33.449  1.00 61.16
ATOM   2720  CG  PHE A1111      38.144  55.601  33.081  1.00 61.16
ATOM   2721  CD1 PHE A1111      39.101  55.397  34.055  1.00 61.16
ATOM   2722  CD2 PHE A1111      38.575  55.820  31.785  1.00 61.16
ATOM   2723  CE1 PHE A1111      40.448  55.431  33.736  1.00 61.16
```

FIG. 6MM

```
ATOM   2724  CE2 PHE A1111      39.917  55.853  31.485  1.00 61.16
ATOM   2725  CZ  PHE A1111      40.845  55.664  32.451  1.00 61.16
ATOM   2727  N   THR A1112      38.080  58.579  33.586  1.00 54.03
ATOM   2728  CA  THR A1112      38.875  59.664  33.030  1.00 54.03
ATOM   2729  C   THR A1112      39.433  59.610  31.628  1.00 54.03
ATOM   2730  O   THR A1112      38.693  59.607  30.694  1.00 54.03
ATOM   2731  CB  THR A1112      40.029  59.942  34.007  1.00100.00
ATOM   2732  OG1 THR A1112      41.181  59.195  33.618  1.00100.00
ATOM   2733  CG2 THR A1112      39.637  59.498  35.430  1.00100.00
ATOM   2736  N   TYR A1113      40.750  59.639  31.504  1.00 39.45
ATOM   2737  CA  TYR A1113      41.514  59.623  30.240  1.00 39.45
ATOM   2738  C   TYR A1113      42.391  60.886  30.057  1.00 39.45
ATOM   2739  O   TYR A1113      42.658  61.611  30.980  1.00 39.45
ATOM   2740  CB  TYR A1113      40.661  59.461  29.000  1.00 60.42
ATOM   2741  CG  TYR A1113      40.682  58.097  28.373  1.00 60.42
ATOM   2742  CD1 TYR A1113      40.003  57.867  27.193  1.00 60.42
ATOM   2743  CD2 TYR A1113      41.168  56.982  29.056  1.00 60.42
ATOM   2744  CE1 TYR A1113      39.776  56.585  26.720  1.00 60.42
ATOM   2745  CE2 TYR A1113      40.938  55.670  28.577  1.00 60.42
ATOM   2746  CZ  TYR A1113      40.231  55.511  27.413  1.00 60.42
ATOM   2747  OH  TYR A1113      39.943  54.290  26.912  1.00 60.42
ATOM   2750  N   ALA A1114      42.852  61.153  28.847  1.00100.00
ATOM   2751  CA  ALA A1114      43.759  62.268  28.741  1.00100.00
ATOM   2752  C   ALA A1114      44.080  62.762  27.312  1.00100.00
ATOM   2753  O   ALA A1114      44.093  63.971  27.052  1.00100.00
ATOM   2754  CB  ALA A1114      45.049  61.857  29.500  1.00 34.32
ATOM   2756  N   GLY A1115      44.317  61.803  26.410  1.00 68.47
ATOM   2757  CA  GLY A1115      44.683  62.024  24.996  1.00 68.47
ATOM   2758  C   GLY A1115      44.399  63.213  24.093  1.00 68.47
ATOM   2759  O   GLY A1115      45.017  63.303  23.036  1.00 68.47
ATOM   2761  N   ILE A1116      43.470  64.088  24.487  1.00100.00
ATOM   2762  CA  ILE A1116      43.066  65.299  23.739  1.00100.00
ATOM   2763  C   ILE A1116      41.700  65.193  23.039  1.00100.00
ATOM   2764  O   ILE A1116      41.049  64.140  23.163  1.00100.00
ATOM   2765  CB  ILE A1116      44.141  65.709  22.727  1.00 87.32
ATOM   2766  OXT ILE A1116      41.280  66.178  22.385  1.00 87.32
TER
HETATM    1  C1  INH I   1      58.113  50.247  12.231  0.00  0.00
HETATM    2  N2  INH I   1      57.524  51.444  12.202  0.00  0.00
HETATM    3  C3  INH I   1      58.303  52.541  12.107  0.00  0.00
HETATM    4  C4  INH I   1      59.686  52.462  12.036  0.00  0.00
HETATM    5  C5  INH I   1      60.234  51.117  12.080  0.00  0.00
HETATM    6  N6  INH I   1      59.434  50.040  12.174  0.00  0.00
HETATM    8  N8  INH I   1      57.877  53.857  12.079  0.00  0.00
HETATM    9  C9  INH I   1      59.057  54.550  11.988  0.00  0.00
HETATM   10  C10 INH I   1      60.219  53.760  11.953  0.00  0.00
HETATM   12  C13 INH I   1      61.633  54.217  11.871  0.00  0.00
HETATM   13  N15 INH I   1      61.632  50.906  12.042  0.00  0.00
HETATM   14  C16 INH I   1      56.477  54.327  12.146  0.00  0.00
HETATM   15  C17 INH I   1      56.258  55.192  13.391  0.00  0.00
HETATM   16  C18 INH I   1      54.809  55.688  13.471  0.00  0.00
HETATM   17  C19 INH I   1      54.371  56.477  12.214  0.00  0.00
HETATM   18  C20 INH I   1      54.670  55.630  10.955  0.00  0.00
HETATM   19  C21 INH I   1      56.121  55.136  10.897  0.00  0.00
HETATM   28  N30 INH I   1      52.949  56.902  12.268  0.00  0.00
HETATM   29  C32 INH I   1      51.997  55.774  12.311  0.00  0.00
HETATM   30  C33 INH I   1      50.531  56.215  12.400  0.00  0.00
```

FIG. 6NN

Kinase catalytic domain structure walkthrough - insulin receptor kinase

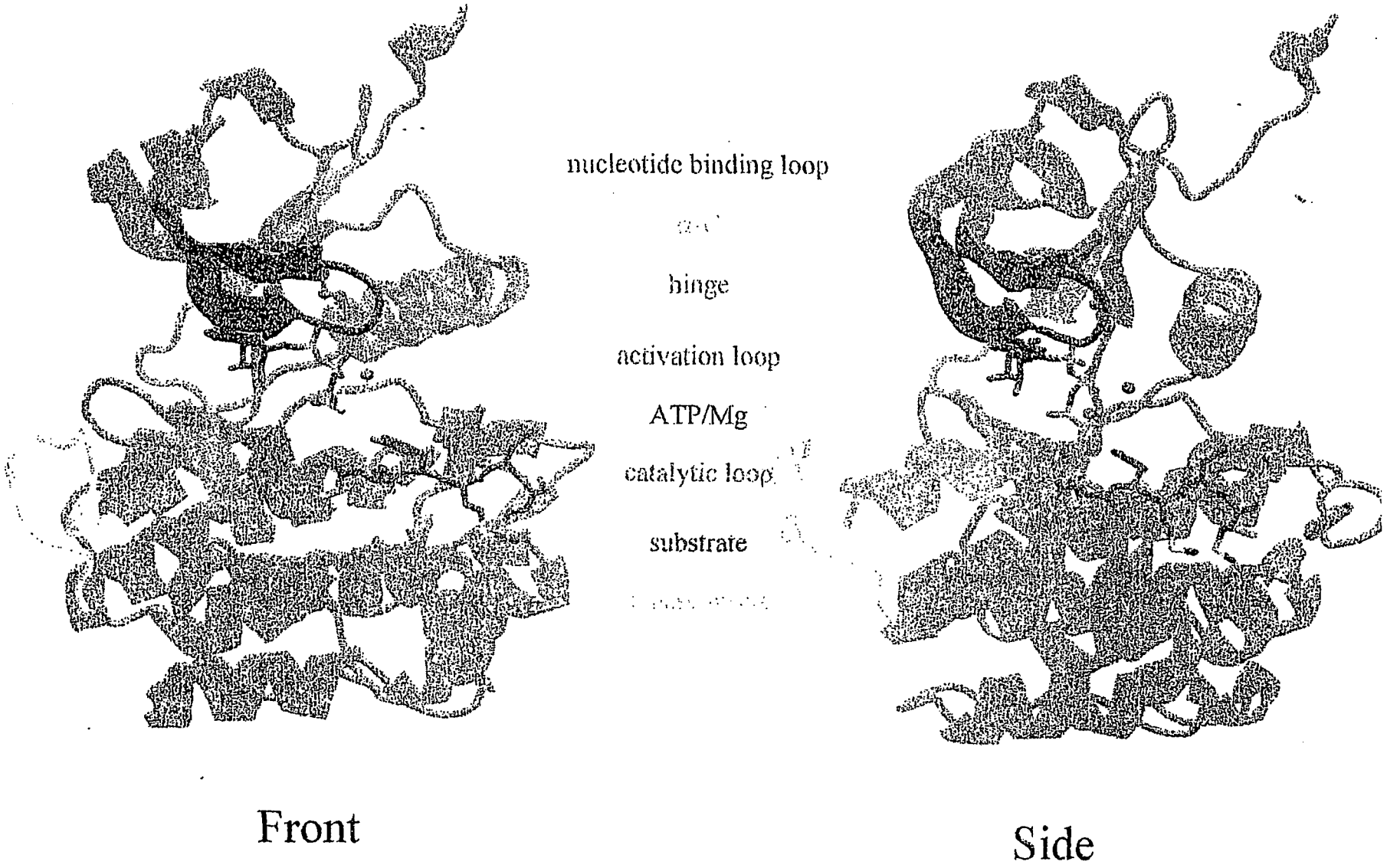

FIG. 7

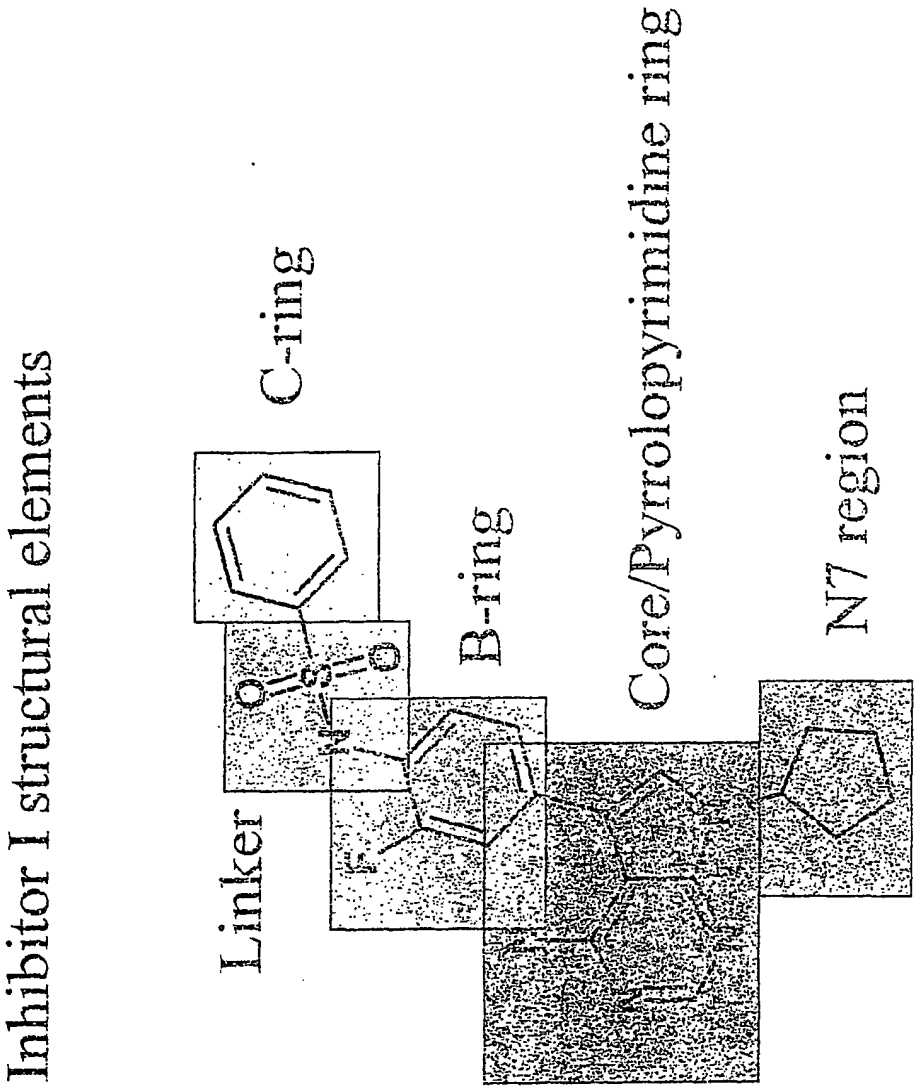
Inhibitor I structural elements
Linker
C-ring
B-ring
Core/Pyrrolopyrimidine ring
N7 region

FIG. 8

BSF421386 binding region

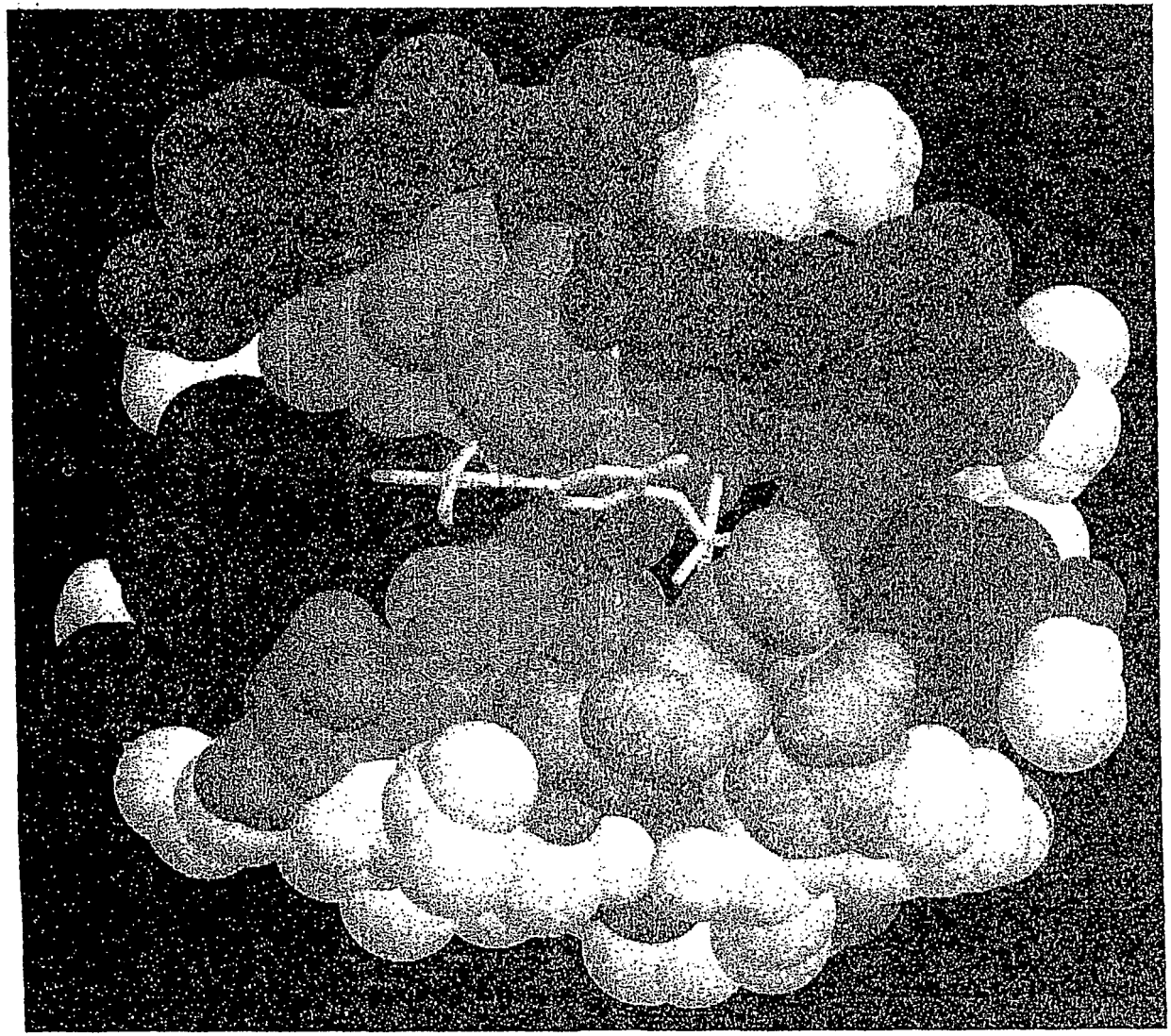

FIG. 9

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(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **BUMP, Nancy, J.** [US/US]; 376 Andover Street, Lowell, MA 01852 (US). **ARNOLD, Lee, D.** [CA/US]; 216 Ruggles Street, Westborough, MA 01581 (US). **DIXON, Richard, W.** [US/US]; 19 Nottingham Drive, Jefferson, MA 10522 (US). **HOEFFKEN, Hans, Wolfgang** [DE/DE]; Dammstuecker Weg 37, 67069 Ludwigshafen (DE). **ALLEN, Karen** [US/US]; 139 Beaver Road, Weston, MA 02493 (US). **BELLAMACINA, Cornelia** [US/US]; 2517 Grove Way #110, Castro Valley, CA 94564 (US).

(74) Agent: **DECONTI, Giulio, A.**; Lahive & Cockfield, LLP, 28 State Street, Boston, MA 02109 (US).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
-- *with international search report*

(88) Date of publication of the international search report:
2 May 2002

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 01/72778 A3

(54) Title: METHOD OF IDENTIFYING INHIBITORS OF TIE-2

(57) Abstract: The present invention relates to polypeptides which comprise the ligand binding domain of Tie-2, crystalline forms of these polypeptides and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Tie-2. The invention also relates to the use of the three dimensional structure of the Tie-2 catalytic domain both alone, or in complex with inhibitors, in methods of designing and/or identifying potential inhibitors of Tie-2 activity, for example, compounds which inhibit the binding of a native substrate to the Tie-2 catalytic domain.

INTERNATIONAL SEARCH REPORT

rnational Application No
PCT/US 01/08853

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C07K14/71 G01N33/68 A61P35/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C07K G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, WPI Data, PAJ, BIOSIS, MEDLINE, CHEM ABS Data, SEQUENCE SEARCH

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 98 07835 A (SCHLESSINGER JOSEPH ;LIANG CONGXIN (US); SUGEN INC (US); TANG PENG) 26 February 1998 (1998-02-26) claims; examples	1-3,87, 88
A	WO 98 41525 A (KNOLL AG ;CALDERWOOD DAVID JOHN (GB); JOHNSTON DAVID NORMAN (GB);) 24 September 1998 (1998-09-24) claims; examples	1,7

☐ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

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"A" document defining the general state of the art which is not considered to be of particular relevance

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"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
5 February 2002	15/02/2002

Name and mailing address of the ISA	Authorized officer
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Form PCT/ISA/210 (second sheet) (July 1992)

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 21-86

Present claims 21-75 relate to a method defined by reference to a desirable characteristic, namely a method for finding a compound which fits into a catalytic domain by use of the atomic coordinates of a crystal of the catalytic domain, and the compounds identified therewith.

The claims cover all methods and compounds having this characteristic, whereas the application provides no support within the meaning of Article 6 PCT and/or no disclosure within the meaning of Article 5 PCT for such methods and compounds. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the method and compounds by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, the no search has been carried out for those claims.

Present claims 76-86 relate to a method defined by reference to a desirable characteristic or property, namely a method of treatment of a tie-2 related condition by administration of a compound found with above mentioned method.

The claims cover all methods having this characteristic or property, whereas the application provides nosupport within the meaning of Article 6 PCT and/or no disclosure within the meaning of Article 5 PCT for such methods. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the method by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, no search has been carried out for those claims.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No
PCT/US 01/08853

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 9807835 A	26-02-1998	US 5942428 A	24-08-1999
		AU 733890 B2	31-05-2001
		AU 4160397 A	06-03-1998
		EP 0931152 A2	28-07-1999
		JP 2001514484 T	11-09-2001
		WO 9807835 A2	26-02-1998
WO 9841525 A	24-09-1998	AU 6829398 A	12-10-1998
		BG 103785 A	30-06-2000
		BR 9808281 A	16-05-2000
		CN 1259950 T	12-07-2000
		WO 9841525 A1	24-09-1998
		EP 0970084 A1	12-01-2000
		HU 0001507 A2	28-10-2000
		JP 2001516353 T	25-09-2001
		NO 994509 A	17-09-1999
		PL 335685 A1	08-05-2000
		SK 125999 A3	16-05-2000
		TR 9902301 T2	21-12-1999
		US 6001839 A	14-12-1999